UNCERTAINTY-OPTIMIZED PREDICTIVE TESTING

FOR A

NUCLEAR WASTE CONTAINER

by

ANDREW JOSEPH WOLFORD

B.N.E. Georgia Institute of Technology
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B.A. Wittenberg University
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Signature of Author _____
Department of Nuclear Engineering
January 21, 1987

Certified by _____
Dr. Norman C. Rasmussen, Thesis Supervisor
McAfee Professor of Engineering

Certified by _____
Dr. Ronald G. Ballinger, Thesis Supervisor
Professor of Materials Science and Nuclear Engineering

Certified by _____
Dr. Ronald A. Christensen, Thesis Supervisor
Research Affiliate and President, Entropy Ltd., Lincoln, MA

Accepted by _____
Dr. Allan F. Henry
Chairman Departmental Graduate Committee

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ANDREW JOSEPH WOLFORD

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Abstract

Techniques of experiment design are developed specifically to address the large uncertainties accompanying 1000 year extrapolation of nuclear waste container penetration by general corrosion.

A methodology is developed which couples a parametric model of general corrosion, laboratory-obtained general corrosion data, and simulated, 'virtual' general corrosion data. Candidate experiments, represented by the simulated data, are investigated for their value in uncertainty reduction at extrapolated times. This methodology is automated in the form of a computer program named UNODEX, which evaluates each candidate experiment from the specified set. The program performs multiple sequential and cumulative evaluations of the candidate experiments to arrive at the optimized experiment design. The program also predicts the time-integrated penetration and uncertainty using predictions of the time-dependent waste container boundary conditions.

The UNODEX methodology is used to investigate waste container penetration and uncertainty as applied to the current salt repository design. Quantitative results are obtained which directly evaluate the role for accelerated life testing at expected conditions.

Thesis Supervisor: Dr. Norman C. Rasmussen

Title: McAfee Professor of Engineering

Thesis Supervisor: Dr Ronald G. Ballinger

Title: Professor of Materials Science and Nuclear Engineering

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DEDICATION

This doctoral dissertation, the culmination and apex of nine and a half years of formal education, is dedicated with love to my dear wife and supporter,

Linda

She was the one, for all those years, that saw my dreams along with me and worked as hard as I did to achieve them. Her courage, faith and strength have sustained our family through the difficult times of trial and her laughter and love have been my deepest joy. Without her encouragement this thesis would never have become a reality.

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1. INTRODUCTION

"He that will not apply new remedies must expect new evils; for time is a great innovator"

- Sir Francis Bacon
Essays II "Of Innovation"

The methodology presented herein for generating "uncertainty-optimized" experiment designs is motivated by and developed in the context of predicting nuclear waste container penetration by aqueous corrosion at long time extrapolations from sparse data. While this application is specific, the methodology is not, and it is anticipated to be a most useful approach to experiment design whenever knowledge in the form of a physical process model and relevant data are available to the experimental planner faced with significant extrapolation in time.

Uncertainty-optimized will be defined here to mean that the product experimental design, if performed, is expected to generate data which will have the most effective and greatest reduction in uncertainty at some desired extrapolated time value such as the design life of a long-lived component. The methodology developed herein is not a new approach to the formal, statistical design of experiments, but rather is a straightforward, nonclassical approach fundamentally rooted in the principles of decision analysis.

The product of this work, then, is a formal methodology which may be used by an experimental planner to design an "uncertainty-optimized" test matrix.

1.1 BACKGROUND

The Nuclear Waste Policy Act of 1982 [57] charges the U. S. Department of Energy with the responsibility of administering the nation's effort for ultimate disposal of High-Level radioactive Waste (HLW) in mined geologic repositories. The primary objective of this national program is to isolate existing and future high-level radioactive waste, generated by defense and commercial endeavors from the human environment. To meet this objective, the U. S. Department of Energy is conducting an extensive program to select three sites for the potential construction of a mined geologic repository, and to develop a facility design which will meet all relevant radiological protection requirements for public health and safety at each of these sites. Ultimately, the goal is to select the superior site from these three candidates.

The philosophy of geologic high-level waste isolation is based on (1) provision of an early radionuclide containment period by the various engineered barriers surrounding the waste, and, after release, (2) reliance on a very long radionuclide transport time to the biosphere by careful selection of a site which has very low groundwater flow rates.

Salt was first suggested as a suitable rock type for waste isolation

in 1957 by the National Academy of Sciences [42]. After more than 30 years site nomination activities of the U. S. Department of Energy [55] have recommended one salt (of three potential) site in Deaf Smith County, Texas. This location is in the panhandle of the state, in a geologic formation called the Permian Basin. This potential site is shown in Figure 1-1.

High-level waste will be disposed of by enclosing spent nuclear reactor fuel (or vitrified liquid defense wastes) in a handling canister, which will in turn be sealed within a thick-walled disposal container*. The disposal container is the outermost sealed metallic vessel which encloses the waste.

Specific federal regulations [59, 58] and design requirements deriving from the Nuclear Waste Policy Act of 1982 [57] have indicated that the waste package is to provide the early radionuclide containment period of 300 to 1000 years. The current salt repository waste package conceptual design relies on a thick-walled consumable disposal container the function of which is to delay corrosion driven failure of the waste package. While designs may be made robust to the uncertainty in corrosion rates by increasing wall thickness, predictions of penetration at 1000 years validated by experimental measurements made over from 1 to

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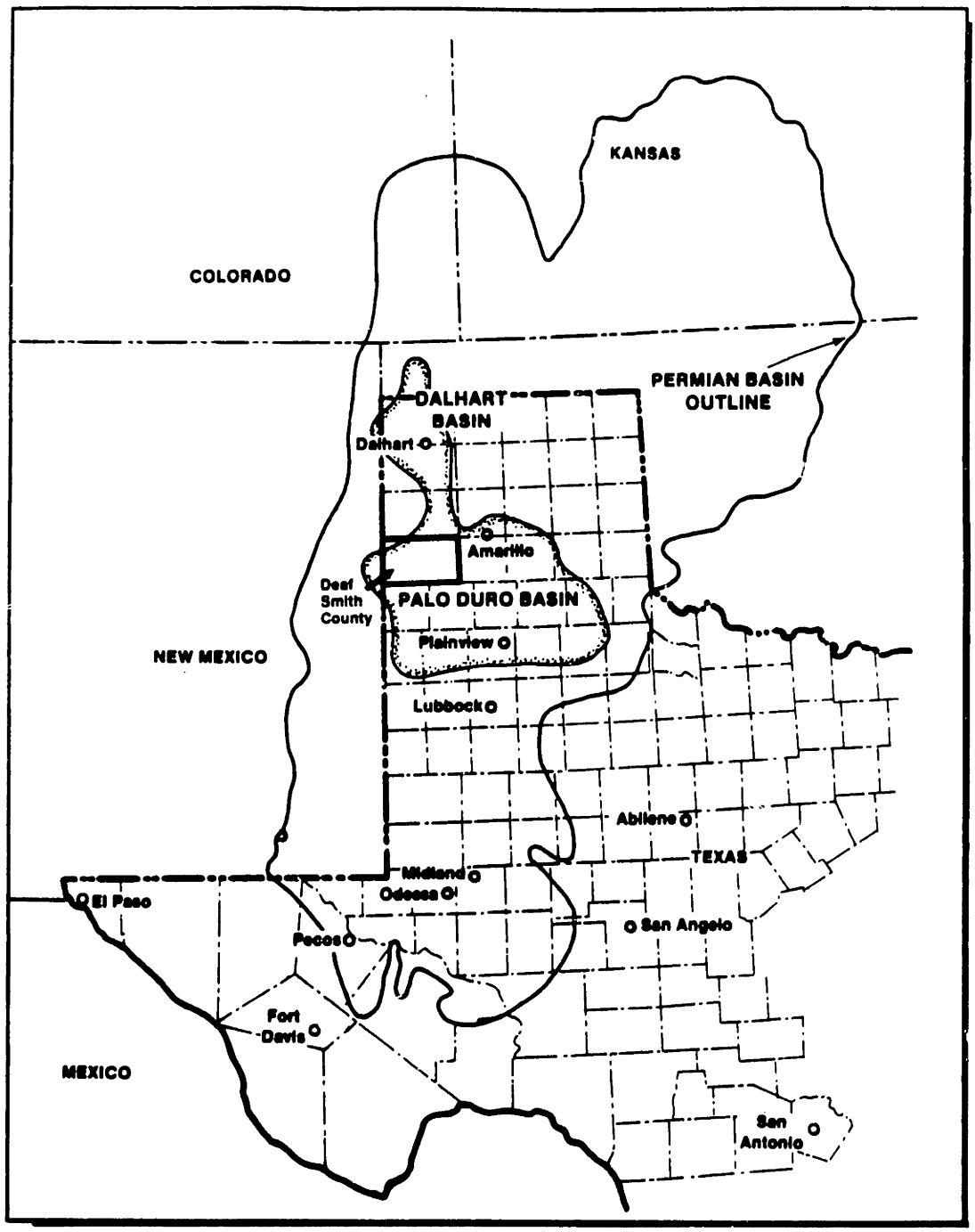
*An equivalent yet obsolete term which has been used in earlier work to refer to this barrier is the "overpack".

Figure 1-1: Location of the Deaf Smith County, Texas Potential Repository Site



5 years will continue to be dominated by the uncertainty in the estimates at those long time extrapolations.

Recognizing the unique difficulties associated with validating performance predictions over time spans of a thousand years or greater, the U. S. Nuclear Regulatory Commission has adopted a qualitative "reasonable assurance" approach to waste isolation compliance, and committed to the use of data generated by accelerated testing:

> For such long-term objectives and criteria, what is required is reasonable assurance, making allowance for the time period, hazards, and uncertainties involved....Demonstration of compliance with such objectives and criteria will involve the use of data from accelerated tests and predictive models that are supported by such measures as field and laboratory tests, monitoring data and natural analog studies [59].

There is much room for general improvement in the field of accelerated testing [7], and reliance on data of this type is likely to introduce new and significant sources of uncertainty in performance assessments. It would be useful at this time to develop the means of quantitatively estimating the "value" of data generated by means of at-condition and accelerated laboratory and *in situ* measurements, *a priori*, in terms of the reduction in estimate uncertainty at the (extrapolated) design life. This is the goal of the following work.

1.2 WASTE CONTAINER DEGRADATION MECHANISMS IN A SALT REPOSITORY

In any experimental investigation of mechanisms of degradation and/or failure, stated or not, there will be some mechanism which is expected to dominate the degradation process over all the others. Usually, the current understanding of the physical processes which drive this dominant mechanism has played a role in the design of the experiment. Generally, however, the role is often subtle, and not formalized enough so as to have become an experimental "strategy".

One goal of this work is to formalize a quantitative evaluation of potential experiments which will most effectively reduce the uncertainty in waste container life prediction. As a necessary first step toward that end, the relevant literature is surveyed to assess the plausible degradation mechanisms which could ultimately lead to a breach of the waste container in service. It is concluded, for the present application (that is, the current waste container design and the present understanding of the repository environment and its projected behavior), the mechanism of general corrosion is the most certain to prevail over the bulk of the package surface. Localized mechanisms such as pitting will likely not be severe, as the steels under investigation do not appear to support localized attack to any penetrations significantly greater than that due to general attack. Although investigators [61] have attempted to induce the mechanism of stress corrosion cracking in simulated repository environments and similar alloy-environment-stress

systems, no evidence of the phenomena has been observed. For this reason, the SCC mechanism has been eliminated from this thesis. And finally, with the weakest of substantiation, the hydrogen assisted failure mechanisms are also excluded from modeling considerations, pending further understanding and specification of the container weldment.

1.3 OUTLINE OF THE PRESENT WORK

By way of organization, the following structure serves to present this thesis. Chapter one is a general introduction to the problem, the simplified strategy of geologic nuclear waste disposal, the motivations which lead to containing the waste in a thick low carbon steel vessels and the uniqueness of making predictions in time, or forecasting, the container behavior and eventual demise.

Chapter two attempts to present a coherent description of the environment which is expected to challenge container integrity, once in service, and a thorough review of the literature for the relevant degradation mechanisms for present container designs.

Chapter three is the methods development section. In this chapter, the hypothesis, logic and approach of the formal methodology for the adaptive experiment design process is described.

Chapter four is the results section of the work, wherein the tools and

techniques are applied to the container life problem. Various assumptions are made and the resulting trends in experiment optimality, and "information value" are presented.

Chapter five, as in any thesis, is the overall summary of the work. As well this chapter contains all the authors own self criticism and hints for future readers. As well, there are several appendices of back matter not suitable, in one way or another, for the running text. These include a computer program listing and documentation, sample input and output and data employed in the studies of chapter four.

2. WASTE PACKAGE CONTAINER DEGRADATION MECHANISMS

2.1 WASTE PACKAGE CONCEPTUAL DESIGN AND RATIONALE

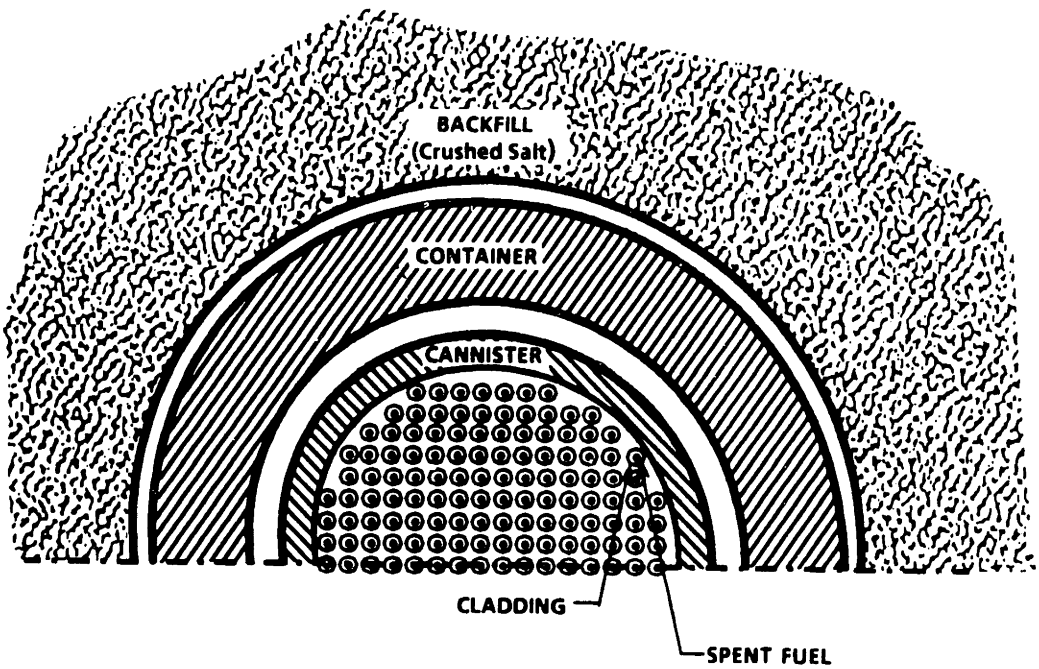
The reference waste package conceptual designs for a repository in salt are described in some detail in the Westinghouse report [63]. The basic features of the waste package design adopted here are repeated for completeness.

Current High-Level-Waste (HLW) isolation concepts in geologic media rely on (1) an early containment period sometimes called the thermal period, followed by a much longer period of rate-limited release to be provided by the engineered barrier system, and (2) a very long transport time (10,000 years) to the biosphere to be provided by the host rock media.

The major components of the engineered barrier system are the waste form, canister, container and backfill--which make up the waste package--and the excavated and structural systems of the underground facility and the materials used to seal them. The waste package is shown conceptually in cross section in Figure 2-1.

In the salt repository, there are no plans for a special backfill material different from the excavated salt, due to its low permeability. The container is therefore assigned a high level of responsibility for containment in the early thermal phase after permanent closure. This

Figure 2-1: Schematic Cross Section of the Waste Package



key allocation of performance to the container serves as a limit on the scope of this work and all efforts will be aimed at projections of container degradation.

Container designs differ slightly in dimension in order to accommodate the different waste form types. As the projected repository inventory fractions of commercial high level waste (CHLW), defense high level waste (DHLW), intact spent fuel (ISF) and consolidated spent fuel (CSF), continue to evolve in time, particularly increasing the anticipated CSF fraction, the CSF container with 12 Pressurized Water Reactor (PWR) assemblies as inventory is adopted for this work.

The disposal container is the outermost sealed metallic vessel the function of which is to delay corrosion-driven failure of the waste package. A conceptual waste package design is illustrated in Figure 2-2. This figure depicts a horizontally-emplaced disposal container which encloses the waste form and handling canister. An emplacement plug is shown sealing the borehole. Table 2-1 accompanies the design and presents the reference features of the CSF (12 PWR) package. Salt repository waste package designs to date have advocated a corrosion allowance concept. The basis of this concept is that in geologic formations the rate of dissolution of relativity low corrosion resistant (active) metals is limited by the oxygen reduction reaction. If this is indeed the case, adequate wall thickness may be incorporated in the

Figure 2-2: Conceptual Waste Package Design

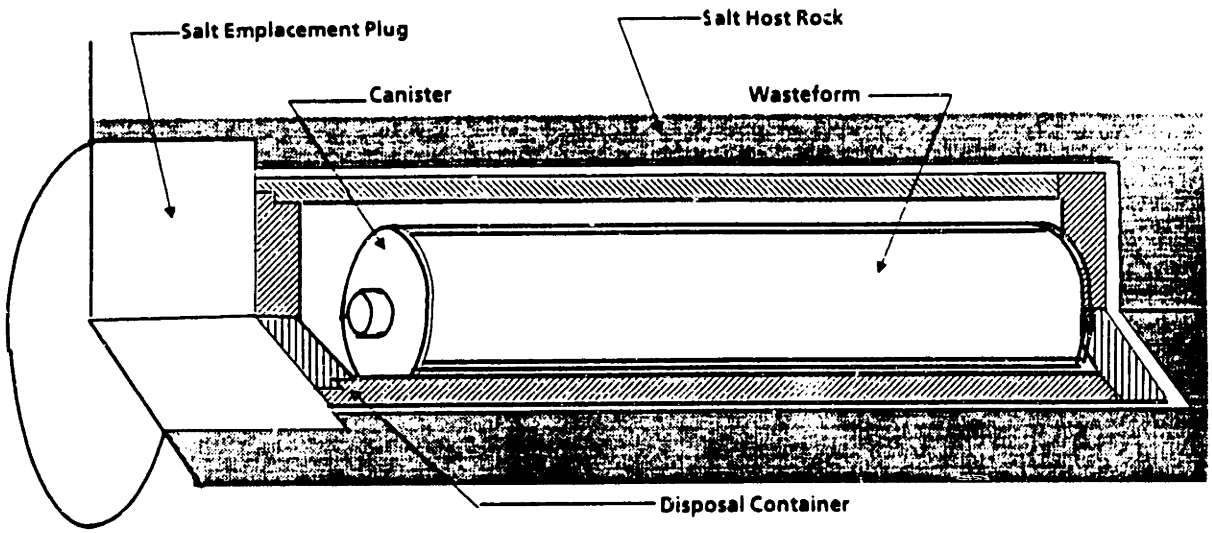


Table 2-1: Reference Features of the CSF(12PWR) Waste Package

Package Thermal Loading	6,600 kW
Package Inventory	5,532 kgU
Repository Areal Heat Loading	14.83 kW/Acre
Waste Form Diameter	62.0 cm
Waste Form Length	400.0 cm
Waste Form Weight	8,390 kg
Container Outside Diameter	84.5 cm
Container Wall Thickness	10.0 cm
Container Head Thickness	18.3 cm
Container Weight	9,250 kg
Total Package Weight	17,640 kg

disposal canister design. Specifically, a castable, fusion-weldable low-carbon steel, which is a slight modification of ASTM A216 grade WCA specification has been specified by the salt repository project [63, 61]. Table 2-2 presents composition and mechanical specifications for the A216 alloy and the recommended disposal container alloy [63]. The modifications reduce the carbon content and eliminate the normalizing heat treatment in an attempt to reduce the formation of martensite and hence vulnerability to hydrogen embrittlement and stress corrosion cracking in any weld heat affected zones.

It is intended, by choosing such a simple alloy for the primary metal barrier material that the alloy will preferentially degrade by the mechanism of general or uniform corrosion, with measurably lower tendency for localized and microscopic mechanisms of perforation such as pitting and environmentally assisted cracking, respectively. This is an assumption which must be supported by further experimental investigation, however.

Other selection criteria which have been considered in the choice of low strength low carbon steel for the container material are:

- Strength Considerations. The minimum yield strength for A216 steel is specified at 206 MPa. The ultimate tensile strength is roughly twice this. Maximum predicted stress at the Deaf Smith site is 17.9 MPa [55].

- Suitability. The data base on low carbon steels is the greatest of all iron alloys, perhaps greater than 100 years.

Table 2-2: Container Material Composition and Mechanical Specifications

	Overpack Material	ASTM A 216 Grade WCA
Elements, %		
Carbon, range	0.15 - 0.20(1)	0.25 (max)
Manganese, range	0.90(1) (max)	0.70 (max)
Silicon, max	0.30	0.60
Sulfur, max	0.65	0.045
Phosphorus, max	0.045	0.04
Residual Elements		
Copper, max	(1)	0.50
Nickel, max	(1)	0.50
Chromium, max	(1)	0.04
Molybdenum, max	(1)	0.25
Vanadium, max	(1)	0.03
Total of these residual elements, max	(1)	1.00
Physicals		
Ultimate Strength, MPa	415-585	415-585
Yield Point, MPa	205	205
Elongation in 2 in., %	22	24
Reduction of Area, %	30	35

(1) The total of these elements shall satisfy the following:

$$0.40 = C + \frac{Mn}{6} + \frac{Cr + Mo + V}{5} + \frac{Ni + Cu}{15}$$

Table 2-2: Container Material Composition and Mechanical Specifications

Although not directly relevant to the application of waste containers in brine environments, familiarity with this alloy and an available expertise helps to eliminate some of the more fundamental research required to rule out esoteric failure mechanisms.

- Fabricability. The alloy specification was developed as an easily castable, fusion-weldable material. This material should present a minimum of difficulty on both the thick-walled casting and remote closure welding operations.

- Ductility. Although not a primary attribute for fabrication, the selected material possesses sufficient ability to plastically deform so as to make it attractive in the event of a handling accident.

- Availability. Large production quantities of the alloy with significant quality control will be required. This should create no problem with the A216 alloy.

- Strategic Materials. In compliance with the siting guidelines [58], construction of the repository should not create any incentive for the future recovery of any material or resource employed and within it.

- Cost Effectiveness. As carbon steel is a very low cost alloy, the cost of the required material resources and fabrication are quite low. Given that the container is a thick-walled vessel, a large amount of raw material is required. Tradeoffs between a corrosion resistant alloy-clad reduced-thickness steel container were performed [63, 62].

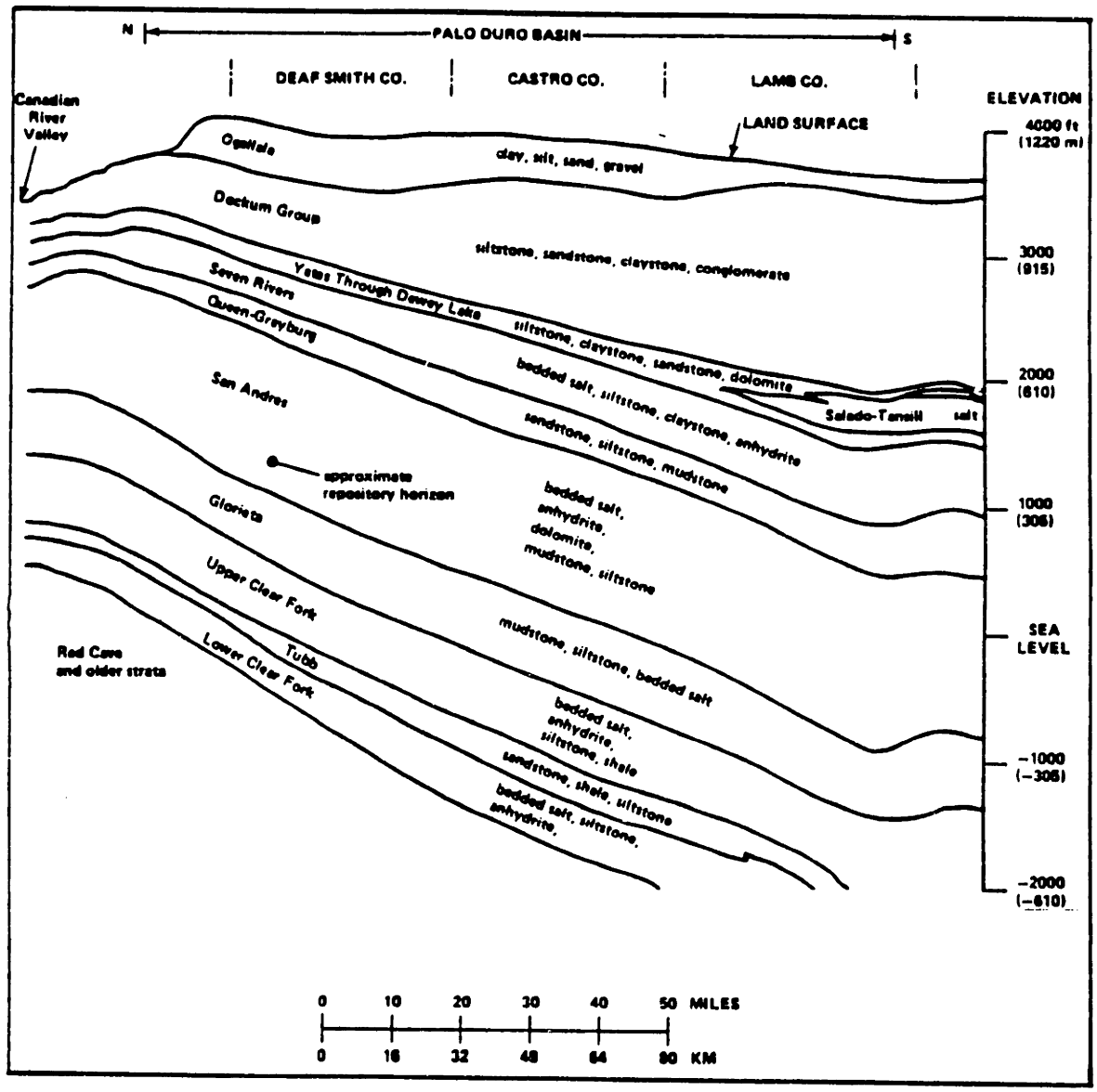
2.2 A DESCRIPTION OF THE RECOMMENDED SALT REPOSITORY SITE

The U. S. DOE has nominated the Deaf Smith County, Texas, bedded salt site for further characterization as a potential high level nuclear waste repository [55]. Figure 1-1 presents the geographic location. As indicated in the figure, the site is located in the Palo Duro Basin, a subunit of the larger Permian Basin. The repository host rock is a

thick layer (approximately 50 meters) of bedded salt within the Lower San Andreas Formation ranging from 700 to 760 meters depth from grade. This depth is referred to as the repository horizon. The Lower San Andreas Formation is subdivided into four layers called Units, and the repository horizon is located in Unit 4. The halite formations throughout the Palo Duro Basin are not pure bedded rock salt, but contain many impurities and interbeds. Hovorka et. al. [29], in compiling core data from 3 test wells near the Deaf Smith Site finds roughly 87 volume percent Halite, 4 percent anhydrite and 9 percent mudstone. In the 50.4 meter thickness of Unit 4, 86 distinct anhydrite beds were observed and more than 100 separate mudstone beds. The San Andreas is overlain by alternating sequences of sedimentary rocks and evaporites consisting primarily of sandstone, limestone, dolomite, shale and anhydrite as indicated in Figure 2-3.

There are three distinct hydrologic units of interest relative to the Deaf Smith Site. The uppermost unit is an unconfined aquifer which is in hydraulic communication with surface water. It is often called the High Plains aquifer, and is composed of the Ogallala aquifer and the Dockum groups. It is very extensive and underlies much of Texas and New Mexico. The repository horizon lies near the mid-depth of the middle unit, which is a large aquitard of some 800 meters in thickness. The deep unit is a brine aquifer composed of much older, fragmented rock.

Figure 2-3: Stratigraphy of the Palo Duro Basin



2.3 THE EXPECTED REPOSITORY ENVIRONMENT

2.3.1 Thermal Conditions

Reference repository conditions have been estimated and compiled by various authors both integral to and independent from the DOE program. The Reference Repository Conditions Interface Working Group [48] (RRC-IWG) have predicted a peak canister surface temperature occurring for a CHLW (25 kW/Acre, 2.16 kW/Package) salt repository of 260°C at 5 years after emplacement. For spent fuel (25 kW/Acre, 0.55 kW/Package) the thermal peak is 160°C at 50 years.

Workers at Brookhaven National Laboratory [50], under contract to the NRC have reviewed the near-field thermal environment. For an equivalent CHLW package design to that employed by the RRC-IWG they cite 264°C as the maximum expected canister surface temperature attained at 3 years post-emplacement.

Cunnane [13] has compiled available information for important factors in the waste package near field environment. Citing the work of McNulty [40], Cunnane indicates for a bedded salt formation the maximum salt-container interface temperature will be between 220°C and 230°C, at approximately 5 years after emplacement. The same analysis for the worst-case salt dome predicts the maximum interface temperature is just under 300°C. It is concluded in this work that the higher dome ambient temperature is the cause of greater peak surface temperatures.

The above, predicted thermal conditions are in good agreement with one another. However, salt thermal conductivity values derive primarily from a single database which was established from a limited number of core samples taken from the Lower San Andreas halite formation. As well, the models used to make the above predictions are fairly simplistic treating the salt media surrounding the waste package as homogeneous and assuming axisymmetric heat transfer. McNulty [40] models the repository as an infinite array of heat sources while the others employ a unit cell approach. This modification tends to increase the interface temperature, however, it is offset by McNulty's use of a correction factor of 1.4 in scaling the laboratory-measured thermal conductivity to reflect realistic in-field values*.

The above analyses employ a 10 year old CHLW package with a loading of approximately 2.2 kW and 10 year old spent fuel with a package loading of 550 W. Both areal heat loadings were 25 kW/Acre. Recent estimates more consistent with the CSF (12PWR) package and an updated areal heat load reflecting horizontal emplacement have been estimated by the Wurm, et. al. TEMP computer program [65]. The results are depicted in Figure 2-4. The peak temperature is 135°C between 3 and 4 years after emplacement.

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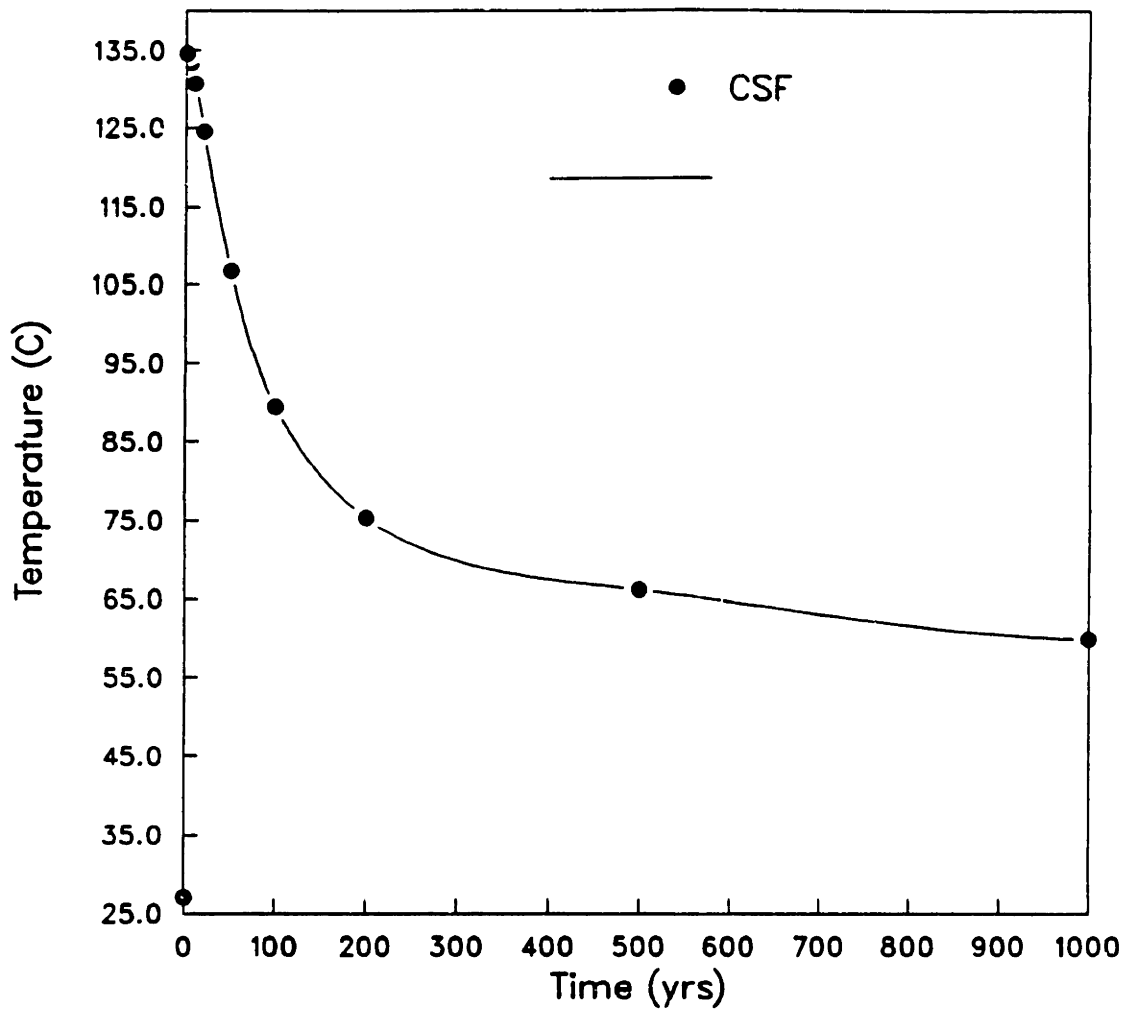
*Laboratory-measured thermal conductivities are lower than *in-situ* measurements, primarily due to stress relaxation upon removal of the salt core specimen.

Figure 2-4: Thermal History of the Salt-Container Interface for the CSF(12PWR) Waste Package Design



There is little reason to argue that the above predictions will be accompanied by significant uncertainty and that detailed *in situ* data will become a necessity in the future, yet a common theme is dictated by these analyses: the salt-container interface will be exposed to a time-at-temperature of greater than 100°C for nearly 100 years.

2.3.2 Water Availability at the Salt Repository Horizon

Natural salt formation can potentially contain three significant types of water sources, the significance of each is formation- and horizon-specific. These sources are:

- Intracrystalline fluid inclusions
- Fluids trapped within halite in grain boundaries
- Interbed water

The brines found as intracrystalline fluid inclusions are found to migrate up an applied thermal gradient. Early investigators, such as Anthony and Cline [1] postulate the migration mechanism is thermally-driven transport, in which brine inclusions become mobile by a process of dissolution and recrystallization at the hot and cold faces of the inclusion, respectively. More recently, Olander and others [43, 1] have suggested brine motion is under thermal control within the crystal, but upon reaching a grain boundary, is controlled by the effective pressure gradient and this fluid then remains confined to the intercrystalline space. This mechanism, thermomigration of halite brine inclusions has received the most attention to date and been the most extensively modeled source of water for waste package performance calculations.

Relatively little empirical data is available to support predictions of brine flow based on thermomigration. However, Jenks and Claiborne [32] have fit an analytical equation for the maximum rates of brine migration versus temperature. The equation relates brine inclusion velocity to temperature and local thermal gradient, thus:

$$\ln \frac{v}{\nabla T_{\infty}} = 0.0656\,T - 0.6306 \qquad (2.1)$$

Where:

$v \equiv$ *Brine inclusion speed (cm/year)*

$T \equiv$ *Bulk temperature of the salt (°C)*

$\nabla T_{\infty} \equiv$ *Bulk temperature gradient in the salt (°C/cm)*

Two models which treat the transport of brine inclusions in the waste package near field environment of a salt repository are the MIGRAIN computer program by Claiborne, et. al. [11] and the BRINEMIG computer program of McCauley and Raines [38]. Both of these models, developed from substantially the same set of working assumptions, avoid explicitly solving the fluid mass and momentum transport equations by evaluating the velocity field throughout the near field region from the phenomenological correlation given above as equation (2.1).

Of any reported analysis, the greatest brine accumulation has been estimated in work supportive of the Salt Repository Project's Draft Environmental Assessment (EA) task. Employing a site-specific temperature profile generated by the Wurm, et. al. TEMP [65] model, the BRINEMIG program predicts 850 liters per package will accumulate in 1000 years for a site located in the Permian Basin formation in Texas. In this analysis, the initial brine content of the site was intentionally overestimated by at least a factor of five. (It can be shown that the sensitivity of total brine accumulation is directly proportional to changes in initial brine content for simple models such as BRINEMIG).

Much lower total brine accumulations have been reported resulting from the MIGRAIN model, (8.50 liters per package [11]), owing to lower initial brine content in the host salt and lower package heat generation rates in the case problem input assumptions.

Sources of likely overestimation of brine accumulation above include assuming the midplane package temperature conditions prevail over the entire package and lack of accounting for the reduction in brine content of the host rock by evaporative processes during the preclosure (operational) phase, nor the time (delay) to resaturation.

Entrapped grain boundary fluids are the other source of included halite water. The transport of this fluid inventory is presumed to

behave as a flow system, under pressure control. Together intracrystalline fluid inclusions and grain boundary fluids in halite of the Deaf Smith County site have been found to contain from 0.1 to 0.8 weight percent water.

The most significant water source from clay minerals is the so called "interbed water", which is the fluid trapped between the sheetlike structures of the smectite clays. The smectite group of minerals are composed of two tetrahedral silica sheets with a central alumina octohedral sheet. The orientation of this sheetlike layer structure is such that there is a slight charge imbalance between the dissimilar silica and alumina units. The incorporation of polar molecules such as water then results in a more uniform electric field across layer boundaries. Hence, the smectites are noted for their ability to easily accommodate great amounts of water between layers. The maximum water content of Unit 4 mudstone (clay structures) is estimated to be 15 weight percent [18, 17]. It should be noted that the differential thermal analysis technique employed in the water release measurements cannot distinguish the small amount of (chemically bound) hydrated mineral water from the interlayer water.

A homogenized average brine content has been estimated by Means [41] by weighting the average halite brine content and average mudstone brine content with the Unit 4 estimates of halite and mudstone mass fractions

mentioned earlier. Results indicate 1.64 total weight percent water averaged over the entire repository horizon.

With regard to brine chemistry it has been found that those brines occurring as intracrystalline fluid inclusions - which possess significantly higher magnesium concentrations due to the greater solubility of the magnesium salts and reduced solubility of sodium chloride within the inclusion - are greatly more corrosive to ferritic steels [61]. Various compositions have been reported based on analyses of fluids prepared and collected in differing ways. Compositions of fluid inclusion brines are often interpreted based upon equilibrium seawater evaporation assumptions (the evaporative processes presumed to have formed the bedded salt structure). Deviations from those expected compositions are explained by participation, to varying degrees, of the inclusion brine in dolomitization* and calcite precipitation reactions. Table 2-3 has been assembled from the various listed sources and presents significant ionic compositions of inclusion brines currently under study in the Salt Repository Program.

In a recent international workshop which was to assess the sources, chemistry and potential movement of brines in salt, participants generally agreed to the following conclusion [12]:

---

*The dolomitization reaction is given by $Mg^{++} + 2CaCO_3 \Rightarrow CaMg(CO_3)_2 + Ca^{++}$. See, for example Berner, R. A., pp. 148-157 for further reading on the theories of sedimentary dolomite formation.

Table 2-3: Ionic Compositions of Fluid Inclusion Brines in Halite (all concentrations in ppm)

Ion	Seawater (1)	Dolomite (2)	Brine B (3)	PPB1 (4)	Brine A (5)	PPB 3 (6)	SSSS (7)
Na^{+}	10,651	63,072	115,000	105,128	42,000	18,650	30,392
K^{+}	380	4,024	15	33	30,000	8,441	6
Mg^{+2}	1,272	15,048	10	115	35,000	42,765	21
Ca^{+2}	400	10,104	900	1,333	600	11,817	904
Sr^{+2}	13	--	15	30	5		
Cl^{-}	18,890	160,720	175,000	163,248	190,000	168,810	45,040
SO_4^{-2}	884	376	3,500	2,735	3,500	129	2,088
HCO_3^{-}	146	--	10	26	700	--	25
Br^{-}	65	--	400	27	400	1,929	--
BO_3^{-3}	--	--	10	--	1,200	--	--

(1) Reference [B-4].

(2) Brine 2 is an observed brine that has participated in dolomitization [C-4].

(3) Brine B is a near-saturated predominantly NaCl brine representative of dissolved bedded salt from the WIPP site. [B-4].

(4) Permian Basin Brine 1 (PBB1) is representative of dissolved bedded salt from the Deaf Smith Co. site, referred to as an intrustion brine [W-2].

(5) Brine A is a representative inclusion brine from the WIPP site [B-4].

(6) Permian Basin Brine 3 is a representative inclusion brine from the Deaf Smith Co. site [W-2].

(7) Serrogate Site Specific Salt (SSSS) is a better attempt laboratory manufacture of Deaf Smith Co. bedded salt. It is improved over PBB1 by being saturated in NaCl at the test temperature of 150 C.

- Intracrystalline fluids are not the major source of water in the bedded formations under study, this is supported by:
    - Inclusions are unlikely to migrate through a grain boundary
    - A temperature gradient threshold exists, below which thermomigration ceases
- Darcy flow is the most probable mechanism for interbed fluid transport
- Compositions of brines resulting from brine-solid salt interaction at elevated thermal conditions are likely to be much more corrosive than those being employed in salt repository testing programs
- Composition of brines arriving at the waste container interface will likely be bounded by the composition and inclusion brine composition.

2.3.3 Stress Conditions

As currently understood there are five significant components contributing to the state-of-stress at the boundary of the disposal container: the overburden pressure which is essentially lithostatic, the hydraulic (brine) contact pressure, vapor and noncondensible gas pressure, thermal stress developed due to the waste form heat generation and residual stress resulting from fabrication. Of these five components, the first three are the least certain from a calculable standpoint, due to the uncertainty in long-term host rock thermomechanical response and brine availability at the interface.

Lithostatic pressure, also called overburden pressure, is site-

specific. For the candidate Deaf Smith County salt site in the Palo Duro basin the repository horizon is between 700 and 760 meters below grade. Initial lithostatic pressure at this depth is has been estimated between 13.8 and 17.9 MPa, vertically [20]. The latter estimate is inferred by direct integration of the density well log. Maxwell et. al. [37] have shown the total stress in the near-field salt is always compressive.

There will be a very short transient response in both the lithostatic loading of the container and the fluid (both gas and liquid) contact pressure. It has been estimated this transient will have a duration of less than one year after emplacement. The lithostatic temporal variations are due to the thermoelastic and mechanical response of the host rock salt. The response of the fluid, increased contact pressure, is due to the increased specific volume and increased vapor pressure of the entrapped brine. The salt will expand as it is subjected to the slow thermal pulse associated with fission product decay heat. As well, halite and clays both flow readily under stress. Creep deformation in the vicinity of the waste container is expected to consolidate the loosely packed material surrounding it and seal the borehole container interface.

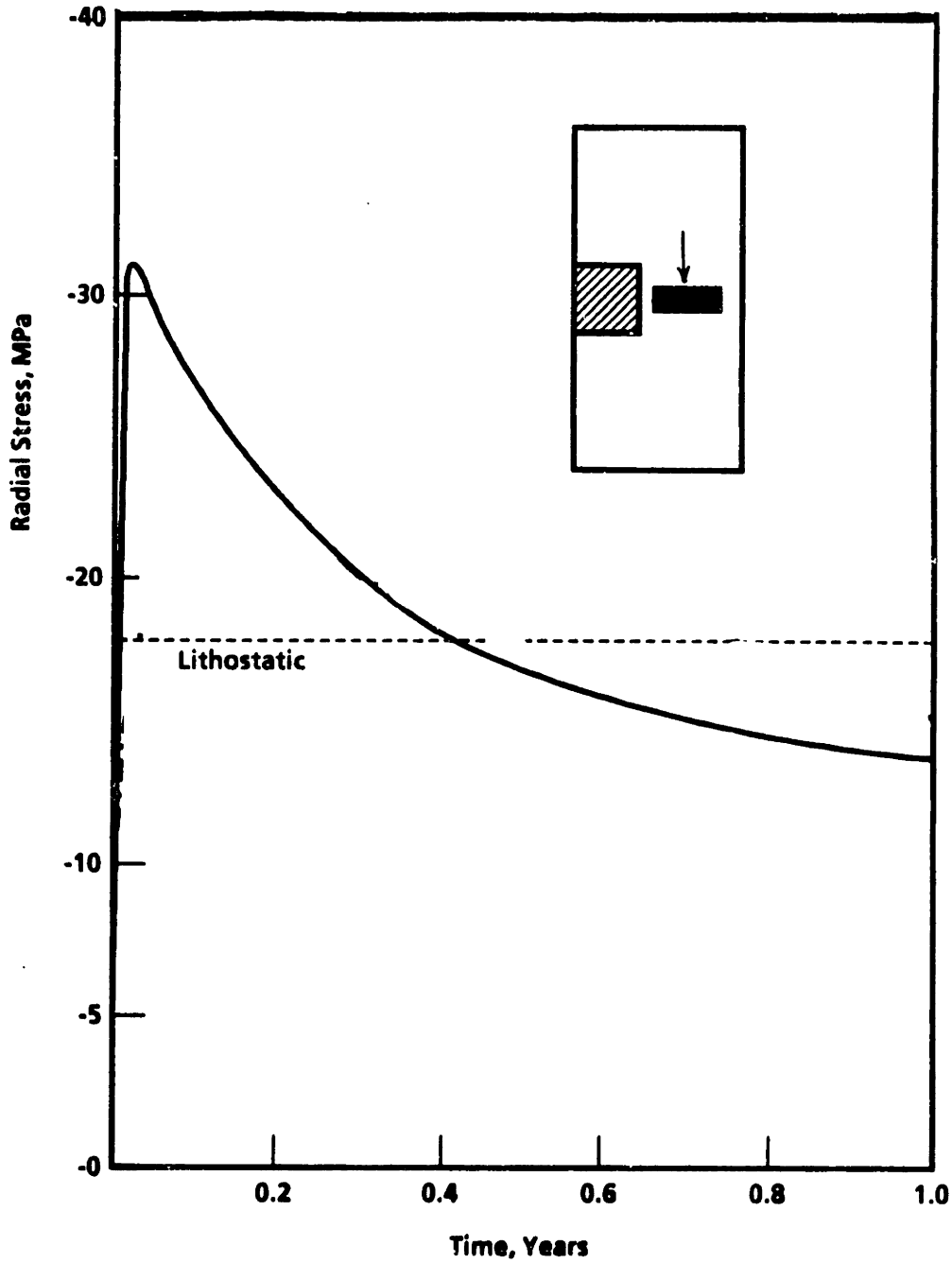
Viscoplastic creep behavior has been investigated for relatively homogeneous bedded halite specimens. Investigators [5, 30] have found a

strong temperature dependence in the proposed constitutive creep rate law. Loken, et. al. [33] have analyzed the lithostatic response for a conceptual repository design with a two-dimensional finite element model of the near field. His findings indicate a short lived transient, due to creep closure in the first year, followed by a gradual approach to initial lithostatic for the lithostatic component of the total stress field. Loken's working assumptions imposed an initial lithostatic stress of 13.8 MPa.

Ghantous [25] has performed an updated evaluation of the thermomechanical repository response to the CSF(12PWR) horizontally-emplaced package design. Results are presented in Figure 2-5 Admittedly [55, p. 6-225], the peak values and decay histories of these stresses are currently poorly defined.

Brine contact pressure and gas and vapor pressures have not been estimated or analyzed in any detail. Potential contact pressures will depend upon (1) the inflow rate and quantity of brine arriving at the borehole-container interface, (2) the rate of creep closure, which determines when and how well sealed the borehole volume is and whether pressures will be relieved due to boiloff of the brine or if the vapor is trapped, and (3) generation of noncondensible gasses; most notably hydrogen from the hydrogen-iron redox reaction.

Figure 2-5: Midplane Container Boundary Stress



It has been pointed out in Section 2.3.2 that the state of knowledge of sources and especially of transport mechanisms for water in the repository environment are rudimentary. A determination of the brine pressure response would be very sensitive to the assumptions of fluid transport models. As well, constitutive laws have not been determined for the impure and heterogeneous bedded salt (and clay) of the Lower San Andres Unit 4 which results in uncertainty relative to the time of borehole closure and estimates of vapor pressures which could be supported by the borehole volume. Finally, corrosion kinetics at the container surface and rates of transport of hydrogen through halite and clay minerals will determine if the borehole volume can support large hydrogen vapor pressures, giving rise to significant container stresses.

In Loken's analysis mentioned above [33] the sum of these fluid pressure transient effects were simplistically accounted for by placing a 25% peak excess radial compressive stress and a 35% peak excess axial compressive stress limit on the transient response. This gave rise to a maximum normal axial stress of roughly 18.0 MPa, while lithostatic was considered 13.8 MPa.

Thermal stresses are expected to be an insignificant contribution relative to the uncertainty in current predictions, and as such have not been included in thermomechanical analyses. Estimated separately from other stress components, employing for carbon steel; a modulus of

elasticity of 2.1×10^5 MPa, thermal expansion coefficient of $1.1 \times 10^{-5}/^{\circ}C$, 2.3 MPa/°C results. Considering that the maximum gradient established through the container is between 1 and 2°C [25], thermal stresses could conservatively contribute from 2 to 5 MPa to overall loading requirements.

Residual stresses are not generally included in the type of analyses presented thus far as it is necessary to know exactly what type of joining technique will be employed in the container design. If the container is to be welded as is indicated in the reference conceptual design [63], it is necessary to establish mechanical properties of the parent plate in the heat affected zone, the effect of any post-weld heat treatment or other stress relief treatment, and the properties of the filler material. McEvily [39] indicates that for butt-type welds in thin plates the stress field is most often compressive near the terminations of the weld (the free edges of the plates) and tensile at the mid-length and mid-depth of the bead. Thick plates behave much less predictably due to the interaction of strains generated in subsequent weld passes. The heating and cooling cycles which would be required of a thick multi-pass weld such as in the waste container can give rise to significant residual stresses, both tensile and compressive, in theory these may approach the yield strength.

2.3.4 RADIATION ENVIRONMENT

Radiation in the waste package near field will be directly determined (and controlled) by design. There should be minimal difficulty associated with calculating the radiation field given the waste form isotopic inventories, geometry and spatial compositions of the salt and backfill materials. A formidable difficulty is encountered in attempting to model the radiation-assisted corrosion effects. Radiation can, in principle, assist corrosion mechanisms primarily via alteration of the electrolyte chemistry.

Fortunately, the radiation field will be significantly attenuated by the thick steel container. It has been suggested by Westerman, et. al. [61] that there is no observable radiation-induced effect on the general corrosion mechanism acting on low carbon steels in repository-like brines at dose rates of 2000 Rad/hour and below.

The results of Jansen, reported in the Deaf Smith Environmental Assessment [55, p. 6-221] indicate the maximum dose rate at the metal-salt interface is 21.2 rad/hour at emplacement for the CHLW package and 32 rad/hour considering the spent fuel source term. This dose rate decays an order of magnitude at some time before 100 years post burial.

2.4 WASTE CONTAINER DEGRADATION MECHANISMS

As has been reviewed earlier in section 2.1 the waste container is a barrier-type component which is functionally to contain its radionuclide inventory by complete enclosure. The container is a passive component from the standpoint that its sole purpose is to provide a time delay to natural geologic transport of the waste. It is doubtful that a waste container design based upon a corrosion allowance could demonstrate compliance with regulatory objectives with any degree of assurance should evidence of the potential for localized, small surface-area penetration (e.g. cracking, pitting) become manifest.

As will be postulated in the following development, the primary challenge to container integrity must be mechanical (e.g. buckling under failure stresses), after sufficient thinning due to general corrosion.

Site selection criteria require evidence to contraindicate past or expected future seismic activity, thereby ruling out the consideration of transient seismic loading of the container. Ruling out this type of loading does not eliminate the catastrophic failure modes linked with environmentally-assisted cracking or buckling under quasistatic loads.

For this review of potential mechanisms, the following categorization will be made. The term macroscopic mechanisms will be used to refer to the processes of bulk metal dissolution, those being general (or

uniform) corrosion, pitting, crevice and galvanic types of corrosion. Microscopic mechanisms will refer to those mechanisms which are operative at the microscopic material level and are nearly always associated catastrophic failure. These are the family of environmentally-assisted crack growth mechanisms to which hydrogen assisted failure (embrittlement) and stress corrosion cracking belong.

2.4.1 Macroscopic Mechanisms

It must be pointed out that conventional wisdom in materials selection for engineering projects would normally reject a low strength low carbon steel for application in an aggressive brine environment. However, predictable, general corrosion is being traded off against greater susceptibility to localized corrosive attack in the case of the salt repository project, due to the inordinately long design requirements and lack of active surveillance over the design life. It is for this reason that although the A216 alloy possesses a fairly comprehensive database, applications similar to the saliferrous environment of the candidate repository are few.

2.4.1.1 General Corrosion

General corrosion involves a reacting surface for which there is no distinct separation of the cathodic and anodic reactions. Both reactions proceed over the entire exposed metal surface. In neutral pH aqueous corrosion processes, the oxygen availability is nearly always the key factor controlling the rate of reaction [22].

The simplest system of ferrous metal dissolution occurs when iron is exposed to a pure water electrolyte. In this case there are two possible reaction paths:

$$Fe + 2H_2O \rightarrow Fe_{2+} + 2OH^- + H_2 \qquad (2.2)$$

$$Fe + H_2O + \tfrac{1}{2}O_2 \rightarrow Fe^{2+} + 2OH^- \qquad (2.3)$$

The first case, equation (2.2), holds under anoxic conditions, and the second when oxygen is present in stoichiometric excess. In most environments of interest the ferrous ion is not stable and the second reaction proceeds further by the Shikkor reaction:

$$3Fe^{2+} + 6OH^- \rightarrow Fe_3O_4 + 2H_2O + H_2 \qquad (2.4)$$

It is illustrative to obtain the overall stoichiometry from equations (2.2) - (2.4), thus:

$$3Fe + 4H_2O \rightarrow Fe_3O_4 + 4H_2 \qquad (2.5)$$

$$12Fe + 4H_2O + 3O_2 \rightarrow 4Fe_3O_4 + 4H_2 \qquad (2.6)$$

This is the classic presentation of the general corrosion of iron, and is very applicable to simple alloys of iron. The feature of interest here is that the thermodynamically stable oxide generated in both cases is magnitite, Fe_3O_4. Also, note that direct comparison between the

anoxic (2.5) and oxic (2.6) consumption of water may be made. That is, oxygen-free corrosion of iron requires four times the water as does corrosion in oxygen-excess conditions.

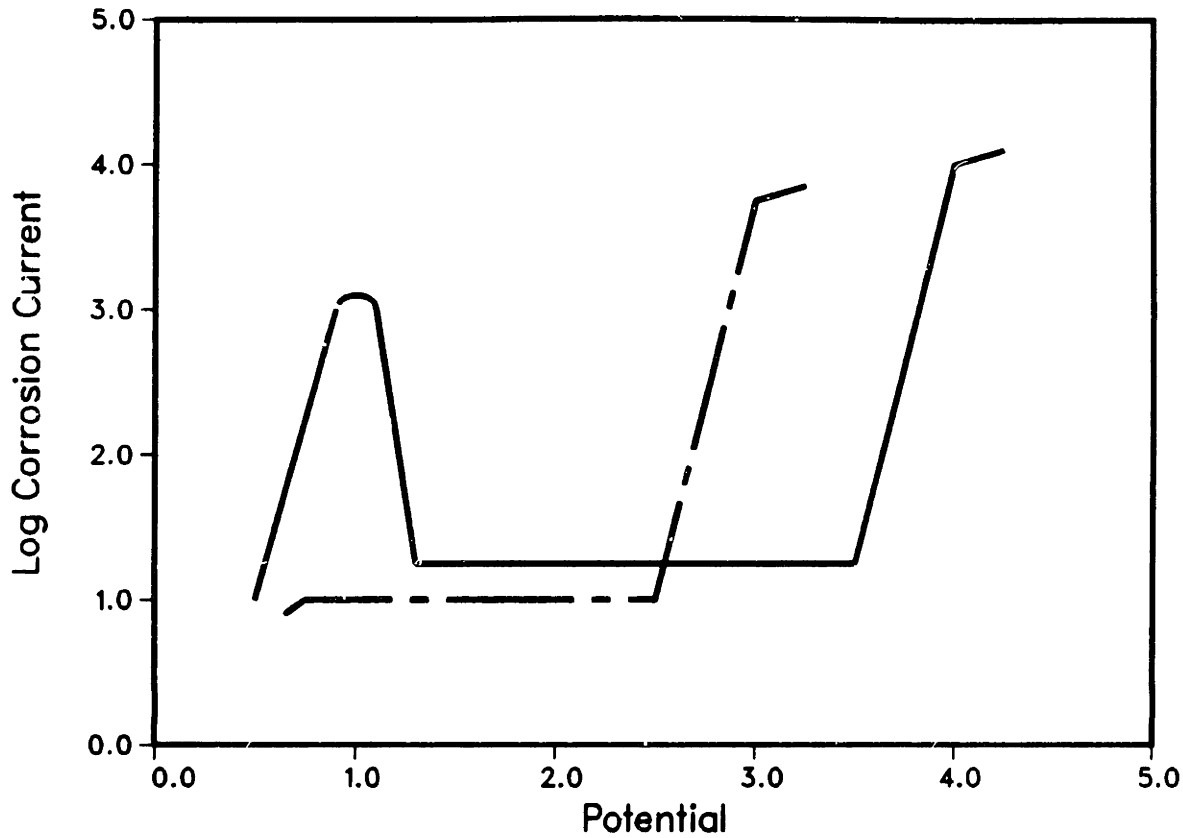
Passivation behavior occurs for numerous alloy-environment systems of interest in engineering applications. The passivation phenomena is observed as a marked decrease in surface reaction rate of an actively corroding metal in certain potential ranges due to the buildup of a protective oxide film. The film inhibits solution-metal contact. Decreases in reaction rate (which is observed as anodic current) of four to six orders of magnitude are common. The formation of a thin (of the order of 30 angstroms), thoroughly-hydrated adherent and protective surface film is implicated as the physical cause of the reduced reaction rate [22, p. 321].

Some metals exhibit passivation-like behavior, though the above definition is not ostensively met. The response may not be as pronounced, though it may still be appropriate to speak of a prepassive, passive and transpassive behavior. Carbon steel magnetite films are porous, reasonably conductive, do not generally contain water of hydration and grow to order-of-centimeter thicknesses. Of prime importance to an understanding of the protective nature of any film is a knowledge of the film composition, structure and relationship to the metal surface upon which it was formed.

Microscopic techniques are useful to identify structure and bulk crystal material properties of the oxide film grown on the metal surface. As well, since the formation and behavior of such films depend on the local thermodynamic state and local electric potential, investigations of these anodic films are also made via electrode kinetics techniques, such as measuring the anodic current response resulting from an externally controlled potential. An idealized anodic polarization curve is depicted in Figure 2-6. The solid line depicts pronounced active-passive behavior, while the chain dash line exemplifies a non-passivating metal. When the external potential is referenced to the reversible electrode potential (the potential at which infinitesimal current would begin to flow) it is called overvoltage and/or polarization.

Foley, et. al. [21] investigated the oxide films formed on iron foils *in situ* with transmission electron diffraction. In all instances the passive films contained gamma-Fe_2O_3 (hematite). Films formed in the prepassive and transpassive (actively corroding) regions of the polarization curve contain the magnetite structure. The measurements were performed in 1N sulphuric acid, and two neutral aqueous environments - 0.1N sodium hydroxide and a buffered (pH=8.5) sodium borate-boric acid solution. In these instances magnetite growth definitively indicated active metal corrosion, even at the observed low corrosion rates.

Figure 2-6: Idealized Anodic Polarization Curve



Park and McDonald [45] report that the growth of porous magnetite films on carbon steels at 200°C and 250°C are parabolic in the early stages of corrosion and after long time obeys linear kinetics. In their particular investigation, a 0.998 M NaCl + 0.001 m $FeCl_2 * 4H_2O$ solution was used. They conclude that the pores of the magnetite film contain an aggressive solution which is maintained by anion (Cl^-) transport and cation (Fe^{2+}) hydrolysis, which eventually reach limiting rates. Using an impedance technique they find that the external imposition of an anodic overvoltage results in an increased rate of corrosion, but the effect decreases with time owing to an increased fractional resistive loss of the overvoltage across the film as it thickens.

Bonnel, et. al. [4] also used an impedance technique to investigate mass transport of oxygen through the porous magnetite corrosion product layer formed on carbon steel in neutral chloride solutions. A rotating disk electrode was employed so as to separate the diffusional component of the oxygen reduction reaction from the total (mixed activation and diffusion controlled) oxygen reduction reaction. They report conclusive evidence providing direct proof of the occurrence of mass transport through porous films and that the overall corrosion reaction studied - carbon steel in neutral chloride media - is rate-limited by the reduction of oxygen under mixed charge transfer and mass transfer control. Dabosi, et. al. [14] support these conclusions in an extension of the same work.

The above survey provides sound generalizations regarding the general corrosion of iron in neutral aqueous solutions. However, the brines present in salt repository environments are significantly more concentrated in dissolved solids, highly conductive and far more aggressive.

Westerman, et. al., [61] have performed an array of gravimetric corrosion tests of carbon steels in repository-like brines. Results to date overwhelmingly indicate severely (one hundredfold) greater corrosion rates for brines containing magnesium. In an attempt to address the correlation of high corrosion rates observed in high magnesium brines, a further series of gravimetric corrosion experiments was performed which varied the magnesium concentration from 0 to 1.7% by weight. These "excess salt tests" (which will be discussed further in Section 4.1.2.) provide significant evidence to support the magnesium concentration dependence of the steel corrosion rate, especially the A216 alloy.

The unique feature of corrosion samples which have been subject to high magnesium brine corrosion is the formation of a thick (2 mm - on both surfaces of a 1.4 mm thick specimen) claylike layer not resembling magnetite. The deposit was not soluable at room temperatures, and resembled a hard clay. An X-ray diffraction spectra of the material corresponded to a complex iron-magnesium hydroxide, $Fe_xMg_{1-x}(OH)_2$. The

endpoint minerals for this mineral series are, for x=1; ferrous hydroxide and for x=0; brucite. The mineral name amakinite is used to refer to any fractional x greater than zero [19].

Since there is no thermodynamic data available for amakinite, reaction paths may only be postulated at this time. Peters and Kuhn [46] have proposed the following magnesium substitution reaction:

$$xMgCl_2 + Fe(OH)_2 \rightarrow Fe_xMg_{1-x}(OH)_2 + FeCl_2 \qquad (2.7)$$

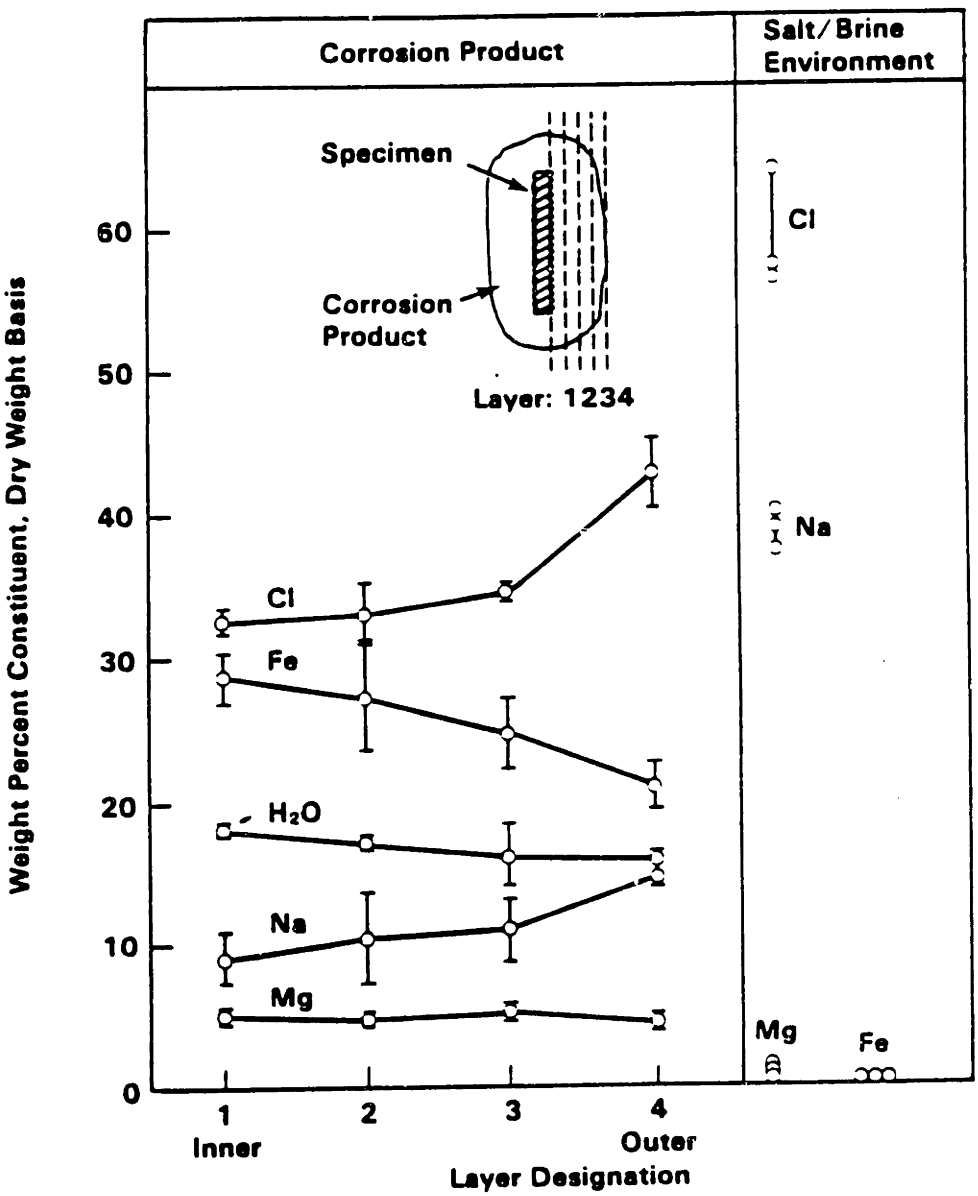
This reaction is consistent with the observed solution pH between 7 and 8 at test termination. If the reaction path involved a metal (magnesium) chloride hydrolysis step;

$$MgCl_2 + 2H_2O \rightarrow Mg(OH)_2 + 2HCl \qquad (2.8)$$

an observable pH drop would be expected. Peters and Kuhn also forward a plausible argument that hydrogen pressures observed in these tests (20 atm.) are at least an order of magnitude too low to stop the forward hydrogen evolution cathodic reaction (see equation (2.5) and (2.6)).

Westerman has also attempted to deduce the composition depth profile of the Amakinite layer by freezing and sectioning. These results are presented in Figure 2-7. Most notable is the uniform magnesium concentration profile and the slight increase in water content near the metal-layer interface.

Figure 2-7: Composition Profile of Amakinite Layer



Further confirmation of the aggressive nature of magnesium-rich solutions is indicated in the work of Pisigan and Singley [47] who after exploring the corrosion rates of mild steel in 22 different synthetic water compositions conclude that corrosion rates of the steels in waters containing significant (20-52 ppm) magnesium concentrations were relatively (50%) higher than the others.

The above early data on corrosion by high magnesium brines and amakinite formation is by no means sufficient to draw any conclusions regarding the reaction path, the kinetics or the long-term behavior of the product layer. However, the following observations are made based on the compiled literature:

- Amakinite formation appears to interrupt the normal magnetite formation from ferrous hydroxide by the Shikorr reaction
- Amakinite is not protective
- Active corrosion proceeds and is only slowed as the amakinite layer grows in thickness, hence the controlling step is likely to be charge transfer (activation)

2.4.1.2 Pitting and Crevice Corrosion

Pitting and crevice corrosion differ from general corrosion only in that the cathodic and anodic reactions are separated. The essential initiator of both is a small stagnant volume of solution in localized contact with the reacting metal. Pitting and crevice corrosion differ from each other only formally in that crevice corrosion occurs in tight crevices and other shielded areas of metal surfaces which are exposed to

electrolytes, while pitting may occur anywhere on a metal surface but requires a pit initiation phase. Pitting attack is extremely localized and varies widely both in the pit number density over the metal surface and in the pit (or cavity) shape. Most often aspect ratios (pit depth/ pit diameter) are high - implying deep, penetrating perforations.

The most universally accepted model of pitting (and crevice) corrosion treats the propagating pit as an occluded anode [22]. Since the occluded cell volume is considered stagnant, the dissolved oxygen which is consumed by the cathodic reduction reaction can only be replaced by the process of diffusion. If the rate of diffusion into the cell falls below the rate of consumption of oxygen within the cell, this imbalance in the redox reactions results in a concentration of dissolved metal cations in the pit. The excess positive charge provides an electric potential gradient which is countered by increased migration of anions, often chloride ions, into the pit. Typically the metal salts (e.g. chlorides, sulfates) then hydrolyze, resulting in more acidic pit conditions. The reaction is autocatalytic if the electric potential driving force is greater than the oxygen concentration gradient caused by depletion. Separation of the anodic and cathodic processes is maintained and cathodic protection of the unshielded metal surfaces continues at the sacrifice of accelerated, localized penetration in the pit.

Pitting occurs in a wide variety of metals and alloys, however it is widely recognized [64] that the most severe pitting attack is associated with strongly passivating metals which exhibit very low general corrosion rates. Pits are more likely to develop in a metallurgically-inhomogeneous metal [56] owing to the different rates of attack upon compositionally-different areas of the surface.

Pit initiation commences when a local breakdown of a protective film occurs. This may result from a local surface imperfection such as an impurity, an emerging dislocation, or a surface scratch which alters, sometimes only momentarily, the rate of metal dissolution. The progression may proceed as described above, once this local anodic area has been established. In pitting corrosion, then, it is often instructive to group metal-environment systems into those in which pit initiation is the overall rate-determining step, and those in which the rate is determined by the rate of pit progression, or growth.

Gupta [27] concludes that in addition to general corrosion, 1040 steel (a low carbon steel similar to A216), depending on pH and sulfide level, will undergo pitting corrosion. He indicates that the most severe attack in neutral environments occurs at sulfide concentrations from 150 to 300 mg/l. These tests were performed at room temperature.

Jelinek and Neufeld [31] indicate that mild steels corroding in de-

aerated neutral bicarbonate-bearing sodium chloride solutions exhibit reduced pitting corrosion rates as a function of temperature up to 90°C, and thereafter, the temperature effect is reversed. Explanations presented in the work implicate an Fe-Cl reaction product in destabilizing the passive film.

Experimental observations in more repository-relevant environments, however, generally indicate much lower vulnerability to pitting corrosion. Canadillas, et. al. [6] have observed shallow, coalesced pits on a fine-grained, structural steel in a high magnesium brine denoted Q-brine. The pits were found to occupy much of the metal surface, and the pit depth was found to approach twice the the penetration due to general corrosion.

These results are consistent with the findings of Westerman [26], also in simulated repository brines, containing high concentrations of magnesium. Westerman observes an initial phase of distinct pitting-like attack, for which the rate eventually slows below that of the general corrosion penetration rate. It has been argued, that in the magnesium-rich brines, the initial pit-like attack is due to the more rapid oxidation of the alpha-ferrite grains [26]

Marsh [35] has postulated a pit progression rate which varies with time raised to the power of 0.49. This was developed for thick carbon

steel containers, but in typical (synthetic) argillaceous groundwaters as opposed to salt brines.

2.4.2 Microscopic Mechanisms

2.4.2.1 Stress Corrosion Cracking

In general, it is thought that the combination of three elements are necessary to induce stress corrosion cracking (SCC): tensile stress, alloy and environment. In fact, it is more general and instructive to speak of environmentally-assisted cracking, of which stress corrosion cracking is a subset.

Observations of stress corrosion cracking for ferritic alloys are found to occur in a tensile stress field of greater than 965 MPa [51], except in extremely potent chemical environments. There are far fewer observances of SCC in low strength steels than in high strength steels.

Relevant reported SCC agents for carbon steels include:

- Nitrates
- Hydroxides
- Carbonates
- Chlorides

Virtually all observations of SCC in low carbon steels are associated with some type of active-passive transition behavior and SCC agents act to shift the potential at the advancing crack tip into the cracking

regime. Beavers, et. al. [2] points out that a close relationship between the polarization (active-passive) behavior and the cracking susceptibility supports the slip dissolution/film rupture model of SCC.

Nitrates are found to be the most potent SCC agents in carbon steel systems. Parkins [44] indicates that not much is known regarding minimum concentrations for attack. Threshold stresses have been measured and tabulated by Parkins, however, and at least 178 MPa is required for the onset of SCC in boiling 1N scdium, potassium, lithium and calcium carbonate solutions. Ammonium nitrate can cause SCC at 92.5 MPa, at 1N concentrations. This may be attributable to the more acidic cation, which results in lower pH.

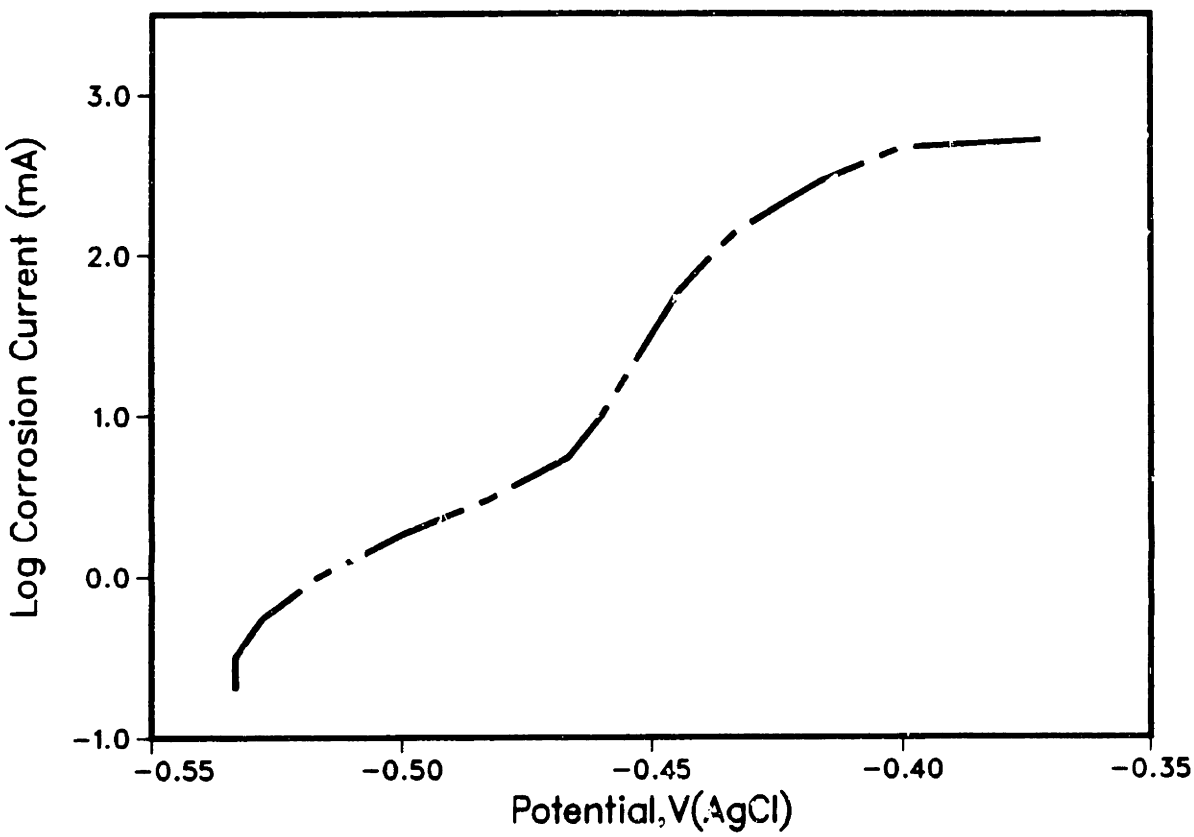
The classic "caustic embrittlement" of locomotive boilers is perhaps the first incidence of SCC of carbon steels. Failure analyses of these boiler components revealed brittle fracture in the region of cold working due to riveting [22], and significant sodium hydroxide deposits, indicating a participating role in the crack propagation. Sodium hydroxide was used as a general corrosion inhibitor in the primary. Temperature and concentration thresholds have been compiled by Beavers, et. al. [2] which indicate at 90°C 24% NaOH is required for SCC, while at boiling (atmospheric pressures) SCC has been observed at 5% concentrations.

Carbonate systems behave similarly to hydroxide systems and occur over a more limited potential range than nitrate systems. Sutcliffe, et. al. [53] has observed the initial evidence of cracking in 22°C, 1N sodium bicarbonate solutions, and below this temperature found no evidence. Parkins [44] has observed a threshold concentration of 0.25N in boiling solutions. All of the above systems were within the pH range of 8 to 10.

It is interesting to present the preliminary work of Pool [26] in Figure 2-8. This anodic polarization trace indicates there is little if any sign of an active passive transition (compare to Figure 2-6). There is a slight indication of a reduction in corrosion current near 1 mA, but this is not sufficient to suspect a transition, or to imply susceptibility.

Strauss and Bloom [52] investigated environmentally- induced cracking in low carbon steels by an array of various ferric oxide slurries at high (316°C) temperature. Individual mild steel capsules were prepared by crimping and welding short lengths of tubing. They report that while concentrated slurries of FeOOH alone did not produce cracking, the susceptibility was markedly changed after the addition of small (mixing with 0.0001M $FeCl_2$) amounts of ferric chloride, and cracking was observed in as little as 3 hours at temperature. The attack was transgrannular, as opposed to all citations mentioned above, and the

Figure 2-8: Anodic Polarization Behavior of A216 Steel in Magnesium Solutions



attack was observed to be preferentially in the plastically-deformed region near the weld or in the martensite-penetrated weld region.

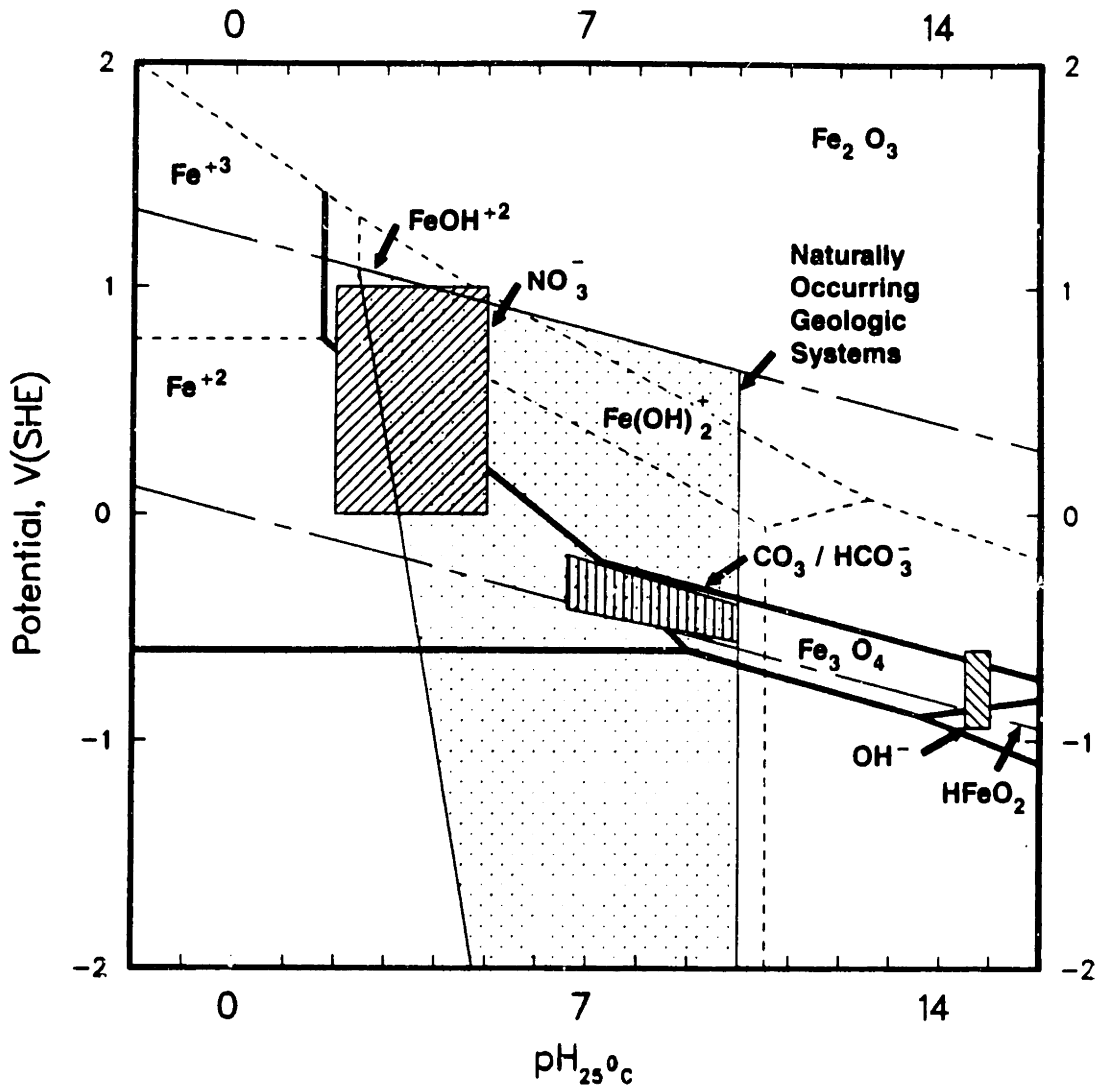
Finally, Ford [23] has assembled a potential-pH (pourbaix) diagram for iron which marks the susceptible regions for nitrate, carbonate/bicarbonate and hydroxide assisted SCC in low carbon steel. This work is presented in Figure 2-9 along with plausible ranges for chloride agent SCC and the region of natural (geologic) system Eh-pH space after Garrels [24].

2.4.2.2 Hydrogen Embrittlement

Hydrogen embrittlement mechanisms have been studied preferentially for the alloyed and high strength steels owing to their much higher susceptibility. High temperature moist environments, corrosion reactions and electrolysis are the major sources of atomic hydrogen. There is some evidence that much of the environmentally activated cracking in ferritic steels is due to the interaction of hydrogen and the advancing crack tip [22]. The majority of models developed thus far have concentrated on slip interference by dissolved hydrogen.

Blundy, et. al. [3] states, for mild steel hydrogen absorption has little embrittlement effect which is substantiated by the vast number of mild steel structures which are cathodically protected in seawater. Cathodic protection of these metals results in favorable environments for charging them with substantial amounts of hydrogen generated by the

Figure 2-9: Potential-pH Diagram for Iron Including Cracking Regimes (After Ford [20])



cathodic hydrogen evolution reaction. The low uptake of hydrogen in these steels is probably due to the low diffusivity of hydrogen in the ferrite grains, which is the major constituent of low strength mild steels.

The greatest concern for embrittlement will be the martensite ingrown weld material, the extent of which, and hence the susceptibility to this type of failure mechanism, must be determined after the benefits of annealing and alloy composition modifications can be assessed.

2.5 SUMMARY

In summary, the previous chapter has outlined the variables of interest in the degradation of waste package containers. The environment has been described and quantified, where possible. Thermal loading requirements have been reduced in the designs reviewed, Peak container-salt interface temperatures of 220°C have been revised by design to 136°C. The early thermal pulse is seen as the most severe in promoting corrosion - greater than 100°C for approximately 100 years. Estimates of fluid (water) availability are unrefined approximations at this time, lacking adequate phenomenological understanding of the basic mechanisms of transport for the most significant sources. Predictions of 8.5 to 850 liters per borehole accumulation in 1000 years have been referenced and indicate this uncertainty. Stress conditions are more tractable and have been calculated based on observed constitutive

relationships for similar bedded halite structures to that found at the Palo Duro site However, discontinuity stresses, due to welding operations could represent the most vulnerable region of the container. This must be determined at some later time when prototype packages can be tested and the behavior of the process weldments can be quantitatively evaluated. The radiation environment has been shown to be sufficiently attenuated by the thick-walled container so as to be considered insignificant in primary effect.

Many investigations of corrosion related degradation mechanisms have been compiled from the literature. Microscopic threshold failure modes have been shown to be of less concern, by lack of observation, in the bulk metal than the mechanisms of general corrosion, pitting and crevice attack. Regions of vulnerability have been identified for container SCC, indicating brine compositions may contain sufficient SCC agents, however the stress and temperature thresholds lie above those expected in the package environment.

Stress corrosion cracking and hydrogen embrittlement, however, must be addressed in the weld zones. Until further fundamental investigations are performed for the weld type and environment of interest this potential "weak link" in the container will not be considered in the analysis of failure prediction herein.

General corrosion is adopted as the only degradation mechanism for the balance of this work, as it is the only mechanism with significant accompanying data.

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3. DEVELOPMENT OF A METHODOLOGY TO SPECIFY UNCERTAINTY-OPTIMIZED EXPERIMENT DESIGNS

3.1 TESTING REQUIREMENTS

It is evident that for nuclear waste container penetration, predictions over such a long design life will be accompanied by significant uncertainty. Testing requirements for a predefined, acceptable uncertainty at a one thousand year extrapolation from data (measurements) taken over hundredths to tenths (at best) of this interval will be undoubtedly great. Practical testing constraints will necessitate some prior strategy if a useful experimental program is to be undertaken. Models of failure are often adopted for this purpose, as is the case wherein lifetime distribution assumptions are made. This avenue is explored in the following section.

In the case where testing of a very reliable component under expected conditions cannot be undertaken due to the long design life, a specific type of testing under more severe environmental conditions is sometimes undertaken. This approach is called accelerated life testing. *Accelerated life testing* (sometimes called predictive testing) will be defined by distinguishing it from *accelerated testing*.

The goal of accelerated testing is to deduce the dominant failure mode for a device by subjecting that device to an environment of increased severity compared with that in-service. Accelerated life testing

differs from accelerated testing in that goal is to measure some reliability parameter of a device at intensified stress levels and from this data predict the performance at normal or expected use conditions. Implicit in the accelerated life testing approach is the requirement that the dominant physical mechanism of failure does not change from the in-service environment to the intensified environment, and the physics of failure must be understood so as to de-rate the intensified environment data correctly. When successful, accelerated life testing is one way to enhance the predictability validation of a process model.

3.1.1 Previous Work

In the following paragraphs, previous work which is relevant to planning experiments for reliability demonstration (that is, the experiment design *and* the amount of data to be gathered) of nuclear waste containers is reviewed. In the context of the long design life goal of 1000 years, these methods are shown to provide insight but fail to establish the detailed methodology to plan an experimental program focused on such long extrapolations. The need for the present work is thus motivated and defined.

3.1.1.1 Lifetime Distribution Approaches and Accelerated Life Testing

One can, in principle, rationalize some particular lifetime distribution for the waste container in the specified repository conditions as an approach to the container failure prediction problem. Using such an assumed model of failure, it is possible, with some very

strong assumptions, to obtain a quantitative measure of the testing requirements which would support reliability predictions with some given probability. This procedure is generally referred to as "testing reliability hypotheses".

Thomas [54], in his creative application of standard reliability hypothesis testing to waste container failure, determines the number of required "container tests" which would be required to accept an hypothesis that the probability of the container lasting some given design life goal is either large, substantiating the high reliability case, or very small, substantiating the low reliability case.

Thomas's approach treats all tests alike, regardless of the control conditions, hence these container tests may be accelerated life tests, or tests at repository-like conditions. Thomas's approach generally indicates the magnitude of testing requirements for such long-time extrapolations and implicitly reveals some of the pitfalls of distributional approaches and accelerated testing. The basic developments are presented here in brief.

Taking Thomas's approach, the framework for the determination is to formulate the test hypotheses:

H_0 The reliability of the container at L years is less than R_0, where R_0 is small, 0.10.

H_1 The reliability of the container at L years is greater than R_1, where R_1 is large, 0.95.

If the failure distribution is presumed to be Weibull* , the reliability for the waste container at fixed time t is given by:

$$R(t) = \exp(-(t/b)^c) \qquad (3.1)$$

with the definitions

$R(t) \equiv$ *Reliability function at time t*

$t \equiv$ *Time*

$b \equiv$ *Characteristic life*

$c \equiv$ *Weibull shape parameter*

The above hypotheses may be restated, mathematically, with the inequalities:

$$H_0 ; \quad R(L) \leq P_0 \qquad (3.2)$$

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*Mann, et. al. [34] indicate that the Weibull distribution has been used to model corrosion-driven failure. However, most derivations of the distribution suggest the failure mechanisms appropriately modeled by the Weibull distribution are those in which the degradation process is active at a number of preexisting flaws, and the time to failure is controlled by the combination of the most rapid degradation at the severest of these flaws. This suggests that the types of corrosion processes most appropriately modeled by a Weibull failure distribution are either localized or microscopic.

$$H_1 ; \qquad R(L) \geq P_1 \tag{3.3}$$

The reliability for a container on test (the reliabilities above were for a container in service), for a test duration D, may be expressed as

$$R_{Test}(D) = \exp(-(fD/b)^c) \tag{3.4}$$

with the definitions

$R_{Test}(D) \equiv$ *Reliability of a container on test*

$D \equiv$ *Reliability function at time (duration) D*

$f \equiv$ *Acceleration factor**

$b \equiv$ *Characteristic life*

$c \equiv$ *Weibull shape parameter*

where Thomas [54] has provided for accelerated container life tests, mathematically, through the acceleration factor, f. This factor transforms the test duration, D (at the accelerated test conditions) to the "equivalent" in-service time (at repository conditions). A value of f greater than unity indicates that the test has been accelerated.

The above transformation in time was a simple scale change, whereas

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*Ratio of effective in-service time to actual time-on-test.

the transformation in reliability is not. The resulting relationship in reliability may be obtained by substituting the characteristic life parameter, b, from equation (3.1) into the container-on-test reliability expression, equation (3.4). Hence,

$$R_{Test}(t) = (R(t))^{q} \tag{3.5}$$

where

$$q = (fD/L)^{c} \tag{3.6}$$

The reliabilities corresponding to the hypotheses may readily be evaluated.

$$R_{Test,0}(t) = (P_0)^{q} \tag{3.7}$$

$$R_{Test,1}(t) = (P_1)^{q} \tag{3.8}$$

Thomas [54] shows that the probability of making a Type I error* that is, accepting H_1 when H_0 is true, is equal to the product of all the success probabilities, where the success probability for a container is given by $R_{Test,0}$ in the case of the Type I error. Thus, the computed Type I error probability for n container tests is

*See, for instance, Chapter 6 in Mann, et. al. [34] for further reading on the theory of testing reliability hypotheses.

$$a = R_{Test,0}^{n} \tag{3.9}$$

and similarly for Type II errors

$$\beta = 1 - R_{Test,1}^{n} \tag{3.10}$$

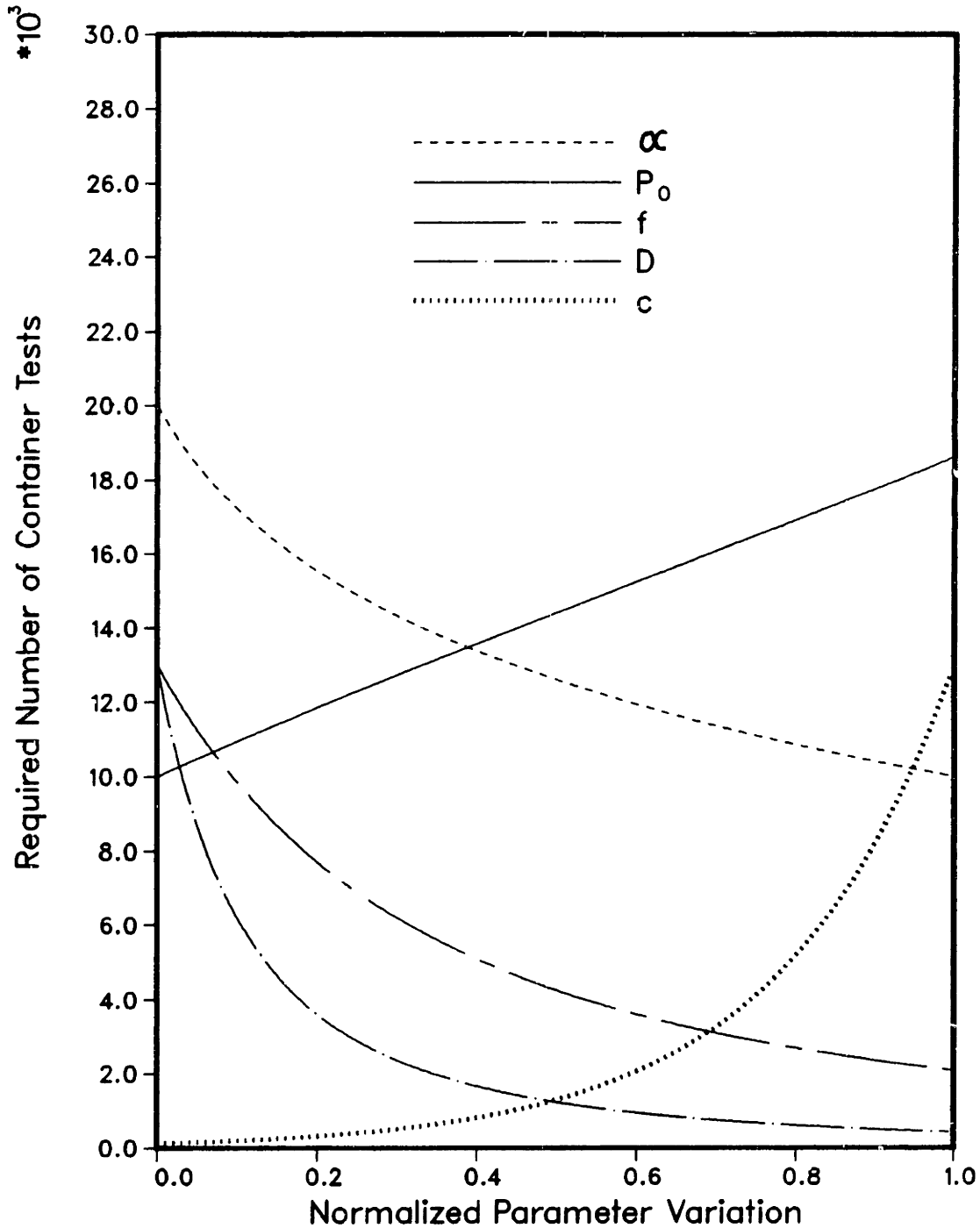
In a straightforward extension of the above, Thomas [54] assigns arbitrary maximum bounds on the probabilities of committing the Type I and Type II errors, a and β, of a^* and β^*, respectively, and develops the upper and lower bounding inequalities for specifying n, the number of tests which must be performed,

$$\frac{\ln (a^*)}{\ln (R_{Test,0})} \leq n \leq \frac{\ln (1 - \beta^*)}{\ln (R_{Test,1})} \tag{3.11}$$

Indeed, if a solution exists for the above inequality, it is customary to select the minimum integer value greater than the lower bound. More complex approaches must be employed when no solution exists, and will not be discussed in this thesis.

Figure 3-1, present the results of the above under various assumed values for the parameters and acceptable probability assignments. As can be seen from the response to parameter variations exhibited, the most severe response is found in the variations of the shape parameter,

Figure 3-1: Test Requirements for Waste Containers Based on a Weibull Failure Model (after Thomas [52])



which was varied from one (Exponential Probability Density Function), and two (Rayleigh PDF). As it approaches the value three (off scale), the number of tests approaches two million. The reduction in tests provided by both f and D are prescribing more measurements at longer effective intervals. Hence, increases in f can be very misleading, as this presumes an exact knowledge of the relationship between the severely overstressed response in the component and the expected service environment behavior, which is seldom achieved. In fact, the most noteworthy "reliable" acceleration factor in engineering applications is observed in routine fatigue measurements, where predictable reductions in component life of 1/15 may be obtained. However, this statement must be qualified, as (1) analogous data at in-service conditions often exists for comparative evaluation, and (2) these estimates of times to failure already have large tolerances (uncertainties) built into the design. A confident acceleration factor of 10 is perhaps optimistic for the waste container.

The short life probability and the probability of making a Type I error, which is sometimes called the producers risk, are seen to have roughly the same effect for the ranges investigated. This has implications regarding the interpretation of applicable containment regulations. It must be cautioned that the approach is only valid for a single mode of failure.

3.1.2 Summary

The above sections indicate that there is quite a lack in the presently available techniques to develop effective test designs for the inherently long-lived component. This is probably due to the pervasive opinion that "Interpolation is generally regarded to be inherently 'safer' than extrapolation"*. There is a need to overcome these deficiencies in the context of the type of prediction problems encountered in the construction of such facilities and engineered components as in the nuclear waste repository described in Chapter 2. The methodology proposed and developed in this thesis provides one means for explicitly treating such long-lived components with a straightforward, albeit nonconventional approach to experiment design. The formal derivations follow in this chapter, while a practical test application is presented in Chapter 4.

3.2 MAXIMUM LIKELIHOOD APPROACH TO UNCERTAINTY ESTIMATION

For the design problem at hand, we are faced with the following:

1. Collection of all data relevant to waste container degradation by general corrosion.
2. Constructing a model which describes this process for the time interval over which the data were obtained.
3. Evaluating the uncertainty of model predictions extrapolated beyond the interval observations.

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*Christensen [8] p. 437.

4. Developing an experiment design methodology to generate data which is expected to reduce model prediction uncertainty most effectively.

The first task, data collection, is discussed in the following chapter, which addresses the application of uncertainty-optimized experiment design to the nuclear waste container life prediction problem. This chapter describes the general foundations of the methodology which was developed to accomplish the second, third and fourth tasks.

3.2.1 The Definition of Failure

One of the classic issues debated in reliability analysis is exactly how to define "failure" for the component under study. This is rather straightforward in the case of the instantaneous failure of a component while under demand. It is not as straightforward in the case in which the component undergoes steady degradation with an associated gradual decline in performance. Often, minimum performance specifications are prescribed and the component is said to have failed when a performance parameter falls below the threshold acceptable value. For the waste container, failure might be defined as container leakage and lifetime the time interval accumulated just prior to the onset of this leakage.

However, for the purpose of this investigation a definition of failure will *not* be postulated. Rather than adopting a single, design-specific definition of container failure (e.g. 4.0 cm of penetration by general

corrosion), methods will be developed considering the cumulative degradation incurred by the component through some specified design life goal. Justifications for making no definition of failure are:

- Any definition of failure under the single mechanism of general corrosion would be design specific, and as such a new definition of failure would be required for each container design iteration (e.g. 4.0 cm of penetration in a 10.0 cm thick container wall may constitute failure while a new cumulative failure penetration would have to be specified for a 12.0 cm container wall thickness).

- The bulk of container degradation and life test data is expected to be derived from material degradation tests, and little is expected to be generated by partial and/or full scale container (component) testing.

- Applicable regulations which normally provide a structure for developing component design requirements are not quantitatively specific and, as such are subject to interpretation.

An advantage of specifying the degradation rate as the dependent variable in the model is that it allows for incorporation of the projected in-service temporal behavior of the independent variables as functional expressions in the degradation rate law, or as discrete constant values over selected time intervals of interest.

3.2.2 Model Development as a Problem in Parameter Estimation

For generality, the degradation rate law (henceforth: rate law) must be able to assume any general functional form. This complicates the task of parameter estimation, as many simplified methods exist for linear models which are inappropriate for nonlinear models. Practically, for high reliability systems and components such as the waste container, knowledge of the physical process of degradation is not precisely known, and the functional form of the selected rate law may be incorrect. The presumption that the rate law chosen *is* correct, when not, may lead to an increase in the 'model, or structural uncertainty' component of the total uncertainty in predicted degradation. In this case a variety of functional forms may be compared by evaluation with the measured data. Furthermore, confidence in the selection of a functional form for the rate law may be heightened, *a priori*, by underpinning the form to that exhibited by similar physical processes.

The working hypothesis for the developments below will be to assume that the postulated model *is* of the correct functional form. This reduces the task of constructing a model suitable for the task of lifetime prediction to a problem of (nonlinear) parameter estimation.

The postulated model of the degradation rate, y, is a function of the independent variables (or, in the language of the experimentalist, the control variables), x_k, and the unknown parameters, b_j.

$$y = f(x_1, x_2, x_3, \ldots, x_K; b_1, b_2, b_3, \ldots, b_P) + \epsilon \qquad (3.12)$$

The notation of capitals to indicate vectors is adopted, hence:

$$X = (x_1, x_2, x_3, \ldots, x_K) \qquad (3.13)$$

$$B = (b_1, b_2, b_3, \ldots, b_P) \qquad (3.14)$$

Thus the degradation rate may be more succinctly expressed as:

$$y = f(X;B) + \epsilon \qquad (3.15)$$

The collection of available, relevant data will be referred to as the *model building database* and is represented as N observations of y and X, the n^{th} of which is:

$$y_n, x_{1,n}, x_{2,n}, x_{3,n}, \ldots, x_{K,n} \qquad (3.16)$$

or just

$$y_n, X_n \qquad (3.17)$$

We will assume that the expected value for the error (vector) is zero and that the errors for individual observations are independent hence, the expected value for y is:

$$E(y_n) = \tilde{y}(X_n;B) \tag{3.18}$$

where the tilda over the y is notation for the estimated value. A reference table of notation is provided in Table 3-1.

Making the assumption of normality, that is, the actual observed data exhibit a random, gaussian error about the expected value for y, the likelihood of observing all the measured data is given by the likelihood function

$$\Lambda(\sigma_n,B) = \prod_{n=1}^{N} (2\pi\sigma_n)^{-N/2} exp \frac{-(y_n-\tilde{y}_n(B))^2}{2\sigma_n^2} \tag{3.19}$$

In the most ideal of situations an individual estimate of the gaussian standard deviation of each measurement in the model building database will be known. In practicality, it is often necessary to presume all the measurements possess a common standard deviation. This disadvantageous assumption may be improved upon pragmatically by employing other estimates of error. Examples of those commonly available even in relatively poor data situations are the calculated (expected) value for the dependent variable and the measured value. Often weighting of some common error value by the reciprocal of one or the other of these may result in an improved fit.

Maximizing the (above) likelihood relative to the parameter set, B, is mathematically equivalent to maximizing the natural logarithm of the likelihood with respect to the parameter set, B, and results in a more manageable system of equations,

$$L(\sigma_n,B) = \ln \Lambda(\sigma_n,B) \tag{3.20}$$

$$L(\sigma_n,B) = C + \sum_{n=1}^{N} exp \frac{-(y_n-\tilde{y}_n(B))^2}{2\sigma_n^2} \tag{3.21}$$

As we are interested in obtaining the maximum of the above log likelihood function, we may arbitrarily assign the constant C to zero without loss of generality.

The system of equations derived by setting the parameter partial derivatives of the log likelihood function to zero is called the system of normal equations. There are P equations in P unknowns:

$$\frac{\partial L(B)}{\partial b_j} = \sum_{n=1}^{N} \frac{(y_n-\tilde{y}_n(B))}{\sigma_n^2} \frac{\partial \tilde{y}(B)}{\partial b_j}, \qquad j=1,P \tag{3.22}$$

If we allow the B' to represent the maximum likelihood solution set of the B parameters,

$$\frac{\partial L(B')}{\partial b_j} = 0 = \sum_{n=1}^{N} \frac{(y_n-\tilde{y}_n(B'))}{\sigma_n^2} \frac{\partial \tilde{y}(B')}{\partial b_j} \tag{3.23}$$

Note also that the error sum of squares, SS(B), which is given by

$$SS(B) = \sum_{n=1}^{N} \frac{(y_n - \tilde{y}_n(B'))^2}{\sigma_n^2} \qquad (3.24)$$

will assume its minimum value when the likelihood is maximum (compare equation (3.21)).

For the normal equations, an approach which leads to iterative solution may be obtained by assuming local linearity in the dependent variable - parameter space. This requires that the initial estimate of the B parameters be close to the solution B' values. Under these restrictions, we may expand a newly-defined function, $z_j(B)$,

$$z_j(B) \equiv - \sum_{n=1}^{N} \frac{(y_n - \tilde{y}_n(B))}{\sigma_n^2} \frac{\partial \tilde{y}(B)}{\partial b_j} \qquad (3.25)$$

as a Taylor series about the solution set B', hence:

$$z_j(B') \simeq z_j(B) + \sum_{m=1}^{P} \frac{\partial z_j(B)}{\partial b_m} (b_m - b'_m) \qquad (3.26)$$

At this point in the solution it is useful to improve upon the notation. Define:

$$\Delta Z_j \equiv Col(z_j(B') - z_j(B)) \qquad (3.27)$$

$$P_{j,m} \equiv \begin{Bmatrix} \frac{\partial z_1(B)}{\partial b_1} & \frac{\partial z_1(B)}{\partial b_2} & \cdots & \frac{\partial z_1(B)}{\partial b_m} & \cdots & \frac{\partial z_1(B)}{\partial b_P} \\ \frac{\partial z_2(B)}{\partial b_1} & \frac{\partial z_2(B)}{\partial b_2} & \cdots & \frac{\partial z_2(B)}{\partial b_m} & \cdots & \frac{\partial z_2(B)}{\partial b_P} \\ \frac{\partial z_j(B)}{\partial b_1} & \frac{\partial z_j(B)}{\partial b_2} & \cdots & \frac{\partial z_j(B)}{\partial b_m} & \cdots & \frac{\partial z_j(B)}{\partial b_P} \\ \frac{\partial z_P(B)}{\partial b_1} & \frac{\partial z_P(B)}{\partial b_2} & \cdots & \frac{\partial z_P(B)}{\partial b_m} & \cdots & \frac{\partial z_P(B)}{\partial b_P} \end{Bmatrix} \qquad (3.28)$$

$$\Delta B_m \equiv Col(b_m - b_m') \qquad (3.29)$$

We may rewrite equation (3.24) as

$$\Delta Z_j = P_{j,m}\, \Delta B_m \qquad (3.30)$$

Thus, the correction vector may be expressed as:

$$\Delta B_m = P_{j,m}^{-1}\, \Delta Z_j \qquad (3.31)$$

The expanded form for a general element of the P^{-1} matrix is

$$p_{j,m}^{-1} = \left\{ \sum_{n=1}^{N} \frac{1}{\sigma_n^2} \left[\frac{\partial y_n(B)}{\partial b_m} \frac{\partial y_n(B)}{\partial b_j} - \frac{\partial^2 y_n(B)}{\partial b_m\, \partial b_j} (y_n - y_n(B)) \right] \right\}^{-1} \qquad (3.32)$$

With an obvious extension in notation an iterative solution may be obtained simply by allowing for successive corrections on the B parameter set. Thus:

$$B_{i+1} = B_i + \Delta B_i \qquad (3.33)$$

until some preset convergence criterion is met. Actually, convergence may be specified for the error sum of squares, on the parameters or preset for each parameter individually.

This local linearization technique has some drawbacks. The most notable is the relatively slow convergence. This is especially true of parameter spaces which possess broad, shallow minima. Various schemes have been suggested to combat the slow approach to convergence. In the cases of the broad, shallow minima, Box* recommends reducing the calculated correction vector if the error sum of squares has been reduced in the iteration, and increasing the correction vector when the error sum of squares has been increased.

As can be noted from the above procedure, the parameter partial derivatives play a key role in arriving at the parameter solution set.

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*For further reading on empirical methods to combat the above and other drawbacks of these problems related to convergence, see Draper and Smith [15].

If these derivatives must be evaluated numerically (as some functional forms mandate), much machine time will be dedicated to this chore alone in a problem of substantial size and with large amounts of data. It is a benefit, from the numerical aspects of the procedure alone, to provide analytical derivatives along with the rate law functional form when possible.

With the formalism for model construction in place, it is now possible to analyze the resultant propagation of error which accompanies prediction in time, or "forecasting" with the model.

3.2.3 Extrapolation and Error Propagation

By way of review, what has been done in the above section is to apply the principle of maximum likelihood to a generalized rate law, y, assuming that the existing set of observations for the rate law, (the *Model Building Database*), is a subset of a population which obeys a gaussian error distribution. The principle of maximum likelihood postulates that the likelihood function, which is defined as the grand product of all these individual distributions at each observation, when maximized by the proper choice of parameters, yields statistics for which the observed state of affairs is most probable.

If the data is very noisy, exhibits much error, the likelihood function will be shallow and possibly possess many local minima, but if the data exhibit a central tendency about the expected value of the rate

law, the likelihood function will possess a sharp peak. Fisher [16] was responsible for calling the curvature of the likelihood function near the maximum the "information value" of the data*.

The matrix given in Equation 3.25 is often called the Fisher Information matrix. When estimates of the B parameter set are obtained by general maximum likelihood techniques as was done above, this matrix is the asymptotic covariance matrix for B'. It can be easily shown that the diagonal elements of this matrix are the individual parameter variances. These mathematical relationships and some approximations are presented as follows.

For any function h which depends upon the random variables $b_1, b_2, \ldots, b_P$,

$$h = f(b_1, b_2, \ldots, b_P) \tag{3.34}$$

we may express the variance, by definition, as:

$$Var(h) = E\left((h - E(h))^2\right) \tag{3.35}$$

We will denote $E(h)$ as $\tilde{h}$ as was done previously. Maintaining

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*This definition of information has led to much confusion with a completely different definition of information arising in the communication engineering discipline (n*Ln(n)) which is more widely familiar. In fact, Christensen [8] advocates the alternative term "evidence" for this curvature about the maximum in lieu of "information"

consistency with the development of maximum likelihood estimates above, we will assume the expected value of the arbitrary function h is approximated well by (is equal to) the function h, evaluated at the maximum likelihood b'_j values.

Once again drawing on Taylor's formula to expand the function of interest, we may approximate the argument of the variance defined above, which we now denote $g(B)$, explicitly noting the functional dependence on the b_j, denoted by the vector B,

$$g(B) \equiv (h - \tilde{h}(B'))^2 \tag{3.36}$$

Hence

$$g(B) = g(B') + \sum_{i=1}^{P} (b_i - b'_i) \frac{\partial g(B')}{\partial b_i} + \sum_{i=1}^{P} \sum_{j=1}^{P} (b_i - b'_i)(b_j - b'_j) \frac{\partial^2 g(B')}{\partial b_i \partial b_j} \tag{3.37}$$

With the relevant partial derivatives

$$\frac{\partial g(B')}{\partial b_i} = 2(h - \tilde{h}(B')) \frac{\partial h}{\partial b_i} \tag{3.38}$$

$$\frac{\partial^2 g(B')}{\partial b_i \partial b_j} = 2 \frac{\partial h}{\partial b_i} \frac{\partial h}{\partial b_j} + \frac{\partial^2 h}{\partial b_i \partial b_j} \tag{3.39}$$

This yields an approximate variance of

$$Var(h) = E((h - \tilde{h}(B'))^2) + 2 \sum_{i=1}^{P} (b_i - b'_i)(h - \tilde{h}(B)) \frac{\partial h}{\partial b_i} +$$

$$\sum_{j=1}^{P} \sum_{i=1}^{P} (b_j - b'_j)(b_i - b'_i) \frac{\partial h}{\partial b_i} \frac{\partial h}{\partial b_j} +$$

$$\frac{\partial^2 h}{\partial b_i \partial b_j} (h - \tilde{h}(B')) \qquad (3.40)$$

With the parameter errors $(b_i - b'_i)$ replaced with σ_{bi} the variance becomes

$$Var(h) = E((h - \tilde{h}(B'))^2) + 2 \sum_{i=1}^{P} \sigma_{bi} (h - \tilde{h}(B)) \frac{\partial h}{\partial b_i} +$$

$$\sum_{j=1}^{P} \sum_{i=1}^{P} \sigma_{bj} \sigma_{bi} \frac{\partial h}{\partial b_i} \frac{\partial h}{\partial b_j} + \frac{\partial^2 h}{\partial b_i \partial b_j} (h - \tilde{h}(B')) \qquad (3.41)$$

Maintaining the original assumptions on h all the $h - \tilde{h}(B')$ terms vanish, yielding

$$Var(h) = \sum_{j=1}^{P} \sum_{i=1}^{P} \sigma_{bj} \sigma_{bi} \frac{\partial h}{\partial b_i} \frac{\partial h}{\partial b_j} \qquad (3.42)$$

Comparing equation (3.42) with (3.32), we note the parameter second partial derivative term missing from the general variance expression, but maintained in the specific case. When the MLE solution to the parameter set is employed, however, this term vanishes. The resultant

P matrix, the inverse of which we will call the "Error Matrix". This matrix is symmetric. The diagonal elements are the individual parameter uncertainties σ_{bj}^2 and the off-diagonal elements are the covariance terms $\sigma_{bi}^2 \sigma_{bj}^2$.

This leads to the standard relationship for evaluating the variance in our arbitrary function h as follows. If we define the row vector S as the P first partial derivatives of h with respect to b_j, the following well known relationship applies:

$$\sigma_h^2 = S\, P_{j,m}^{-1}\, S^T \qquad (3.43)$$

Note the individual observation standard deviations, σ_n^2, may be (and will often have to be) assumed equivalent (homogeneous variance) and will just become a constant scalar multiplier. The appearance of the second partial term in equation (3.21) arises from the solution technique for the MLEs which was used and the particular assumption of a gaussian error distribution. In fact, this term is ultimately dropped from the numerical algorithm for error propagation as it is found to hinder convergence, and, within the accuracy of the data employed in the application to waste container degradation, is unnecessary.

For an extremely high reliability component, we are concerned with obtaining an estimate of the time-integrated degradation and the

associated uncertainty at some target design life goal. Furthermore, it is assumed that we possess some knowledge of the in service environment. Specifically, we must have a projection of the time dependent behavior of the independent variables in the rate law model.

We will define the target design life goal as t_d and the integrated degradation to the component as the accumulated damage, D. Hence, evaluated with the maximum likelihood parameter solution set:

$$D(B') \equiv \int_0^{t_d} y(X(t);B')dt \tag{3.44}$$

The accumulated damage becomes the relevant function for which we must evaluate the uncertainty. The relevant parameter partial derivative is given by:

$$\frac{\partial D(B')}{\partial b'_j} = \int_0^{t_d} \frac{\partial y(X(t);B')}{\partial b'_j} dt \tag{3.45}$$

The uncertainty in the accumulated damage at extrapolated design life t_d is given by:

$$\sigma_D = \sum_{j=1}^{P} \sum_{m=1}^{P} \frac{\partial D(B')}{\partial b'_j} \frac{\partial D(B')}{\partial b'_m} P^{-1}_{j,m} \tag{3.46}$$

Hence a 2σ equitailed confidence interval for D is:

$$(D - 2\sigma_D \ , \ D + 2\sigma_D) \tag{3.47}$$

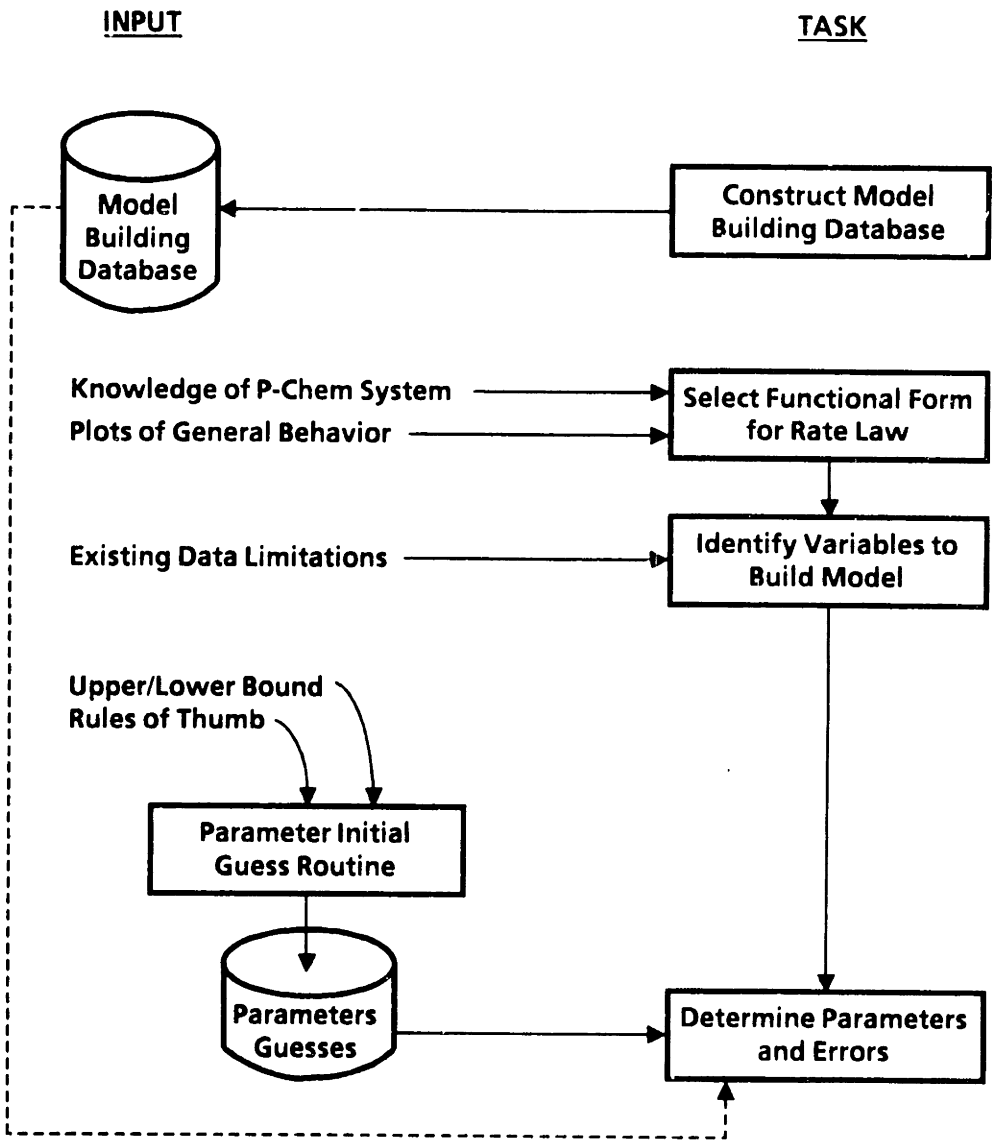
3.3 EXPERIMENT DESIGN: APPROACH

With both model development and uncertainty prediction techniques theoretically established in the previous sections, the overall logic for the design of uncertainty-optimized experiments can now be presented.

Figure 3-2 presents a simplified logic diagram outlining the steps in model development, including the pragmatic concerns under the column labeled "Input". As has been mentioned before (task 1 of section 3.2) the *model building database* must be constructed from all data relevant to the degradation process. This database must specifically include the degradation rate behavior at explicit times and corresponding control variable information. The model building database is the singly most important input required, hence a rigorous evaluation of the *relevance* of the data to the expected in-service environment must be performed. At this point, however, no data should be ruled out for reasons other than relevancy. The database should be pruned of "bad" data points only after its individual measure of error may be compared to estimates of deviation for the total population of data.

A rate law functional form(s) must be specified. As has been mentioned numerous times, this step requires sound underpinning to

Figure 3-2: Logic Diagram for Model Development



theoretical expectation. Knowledge of the physical-chemical system must be brought to bear on this identification. In recent studies of the reliability of various nuclear power plant systems and components, the idea of component "aging" while in service has enjoyed much interest. Carfagna and Gibson [7] have reviewed equipment aging theory and technology. They present a variety of general rate law functional forms for component aging, and discuss the applicability of these to the aging (degradation) of materials and devices in service in the nuclear industry. Based on this review, two general rate laws (Arrhenius and Eyring) are presented in Table 3-2.

It is not surprising that successful application of such first-principle models are usually achieved for rather simple, thermally-controlled degradation processes which are frequently chemical in nature. These formulations represent the endpoint of simplicity in degradation theories, and their unmodified use is likely to be the exception, not the rule. Most often, the rate law will be application-specific and the device and degradation phenomena will dictate the type and sophistication of the model employed.

After specifying the rate law functional form, the next task is to determine the important independent variables from which the model will be constructed. Often, in standard statistical analyses (e.g. regression analyses) these tasks are reversed. The formalism here

Table 3-2: The Arrhenius and Eyring Rate Law Models

THE ARRHENIUS MODEL

The Arrhenius model is usually applied to thermal aging in the form

$$R = B(t)e^{\phi/kT}$$

where:

R = Reaction rate

B(t) = Prefactor (usually a function of time)

ϕ = activiation energy (eV)

k = Boltzmann's constant (0.8617×10^{-4} eV/K)

T = absolute temperature (K)

THE EYRING MODEL

The Eyring model provides a thermodynamically more correct formulation and may include additional (nonthermal) stress terms.

$$R = aT^{w} \exp \frac{b}{kT} \exp \left[\left(c + \frac{d}{kT}\right) f(S)\right]$$

where:

R = Reaction rate in the presence of applied stress

k = Boltzmann's constant

T = absolute temperature

a, b, c, d and w = experimentally determined constants independent of time, temperature, and stress

f(S) = a function of the applied stress

S = the applied stress

requires that the overall physical mechanism be understood first and the functional form of the rate law be accepted as correctly representing the physical process.

The independent variables are to be functionally incorporated into the rate law through modifying the value of some "characteristic dimension" of the system. This means, for example, that the solution chemistry, measured for instance as pH, might be incorporated into an Arrhenius rate law by altering the activation energy term. The activation energy term is thereby viewed as a "characteristic dimension" of the process model.

The importance of making a prudent initial guess for the parameter solution set cannot be overemphasized, especially in light of the local linearity assumption made in developing the algorithm for solving for the parameter correction vector. Utility computer programs may easily be written to facilitate exploration of the parameter space interactively. This is also the stage to incorporate engineering/scientific judgement in the overall model development scheme. This may take the form of constraint on parameter ranges to within bounding estimates of the rate behavior.

Still referring to the logic diagram Figure 3-2, the final calculations can be made and the model parameter solution set

determined, based on the theoretical approach presented in section 3.2. The fitting algorithm which solves the normal equations for the parameter solution set will be discussed in more detail below.

3.4 EXPERIMENT DESIGN: SIMULATION AND EVALUATION

Many mathematical/statistical techniques exist for the design of optimal experiments. The numerous techniques used in optimality theory for the design of experiments differ primarily in the distributional assumptions and the specific optimality criteria.

Harper [28] surveyed various classical methods of designing fixed, preplanned optimal experiments. In his thesis, Harper [28] proposes the use of algorithms which adapt the classical approaches of optimality theory to sequential experiment design. That is, design techniques which allow modification (or updating) of the fixed design after some fraction of the data has been obtained. This work was developed in the context of the "shelf life" problem and involved a short-lived perishable product as compared to a high reliability engineered component. Also, the above work was developed only for interest in binary acceptance data presumed to obey a logistic model.

The work presented herein is also an adaptive approach to experiment design but is unique in that there is never any "fixed" experiment design, generated *a priori*, upon which to iterate. Rather, the state of knowledge is assessed, by model construction from the model building

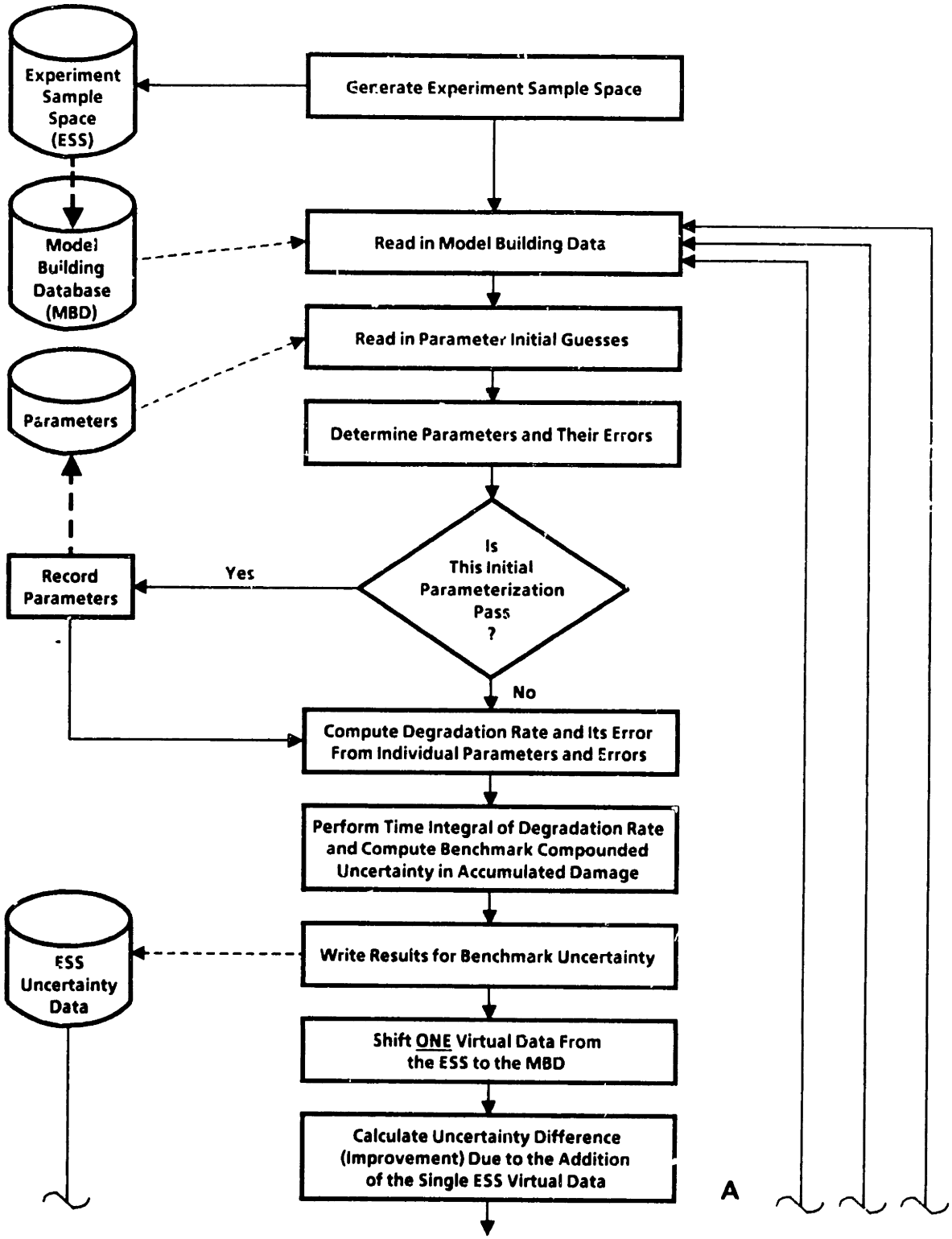
database, and a large collection of potential experiments are individually evaluated for their contribution to uncertainty reduction at the design life goal.

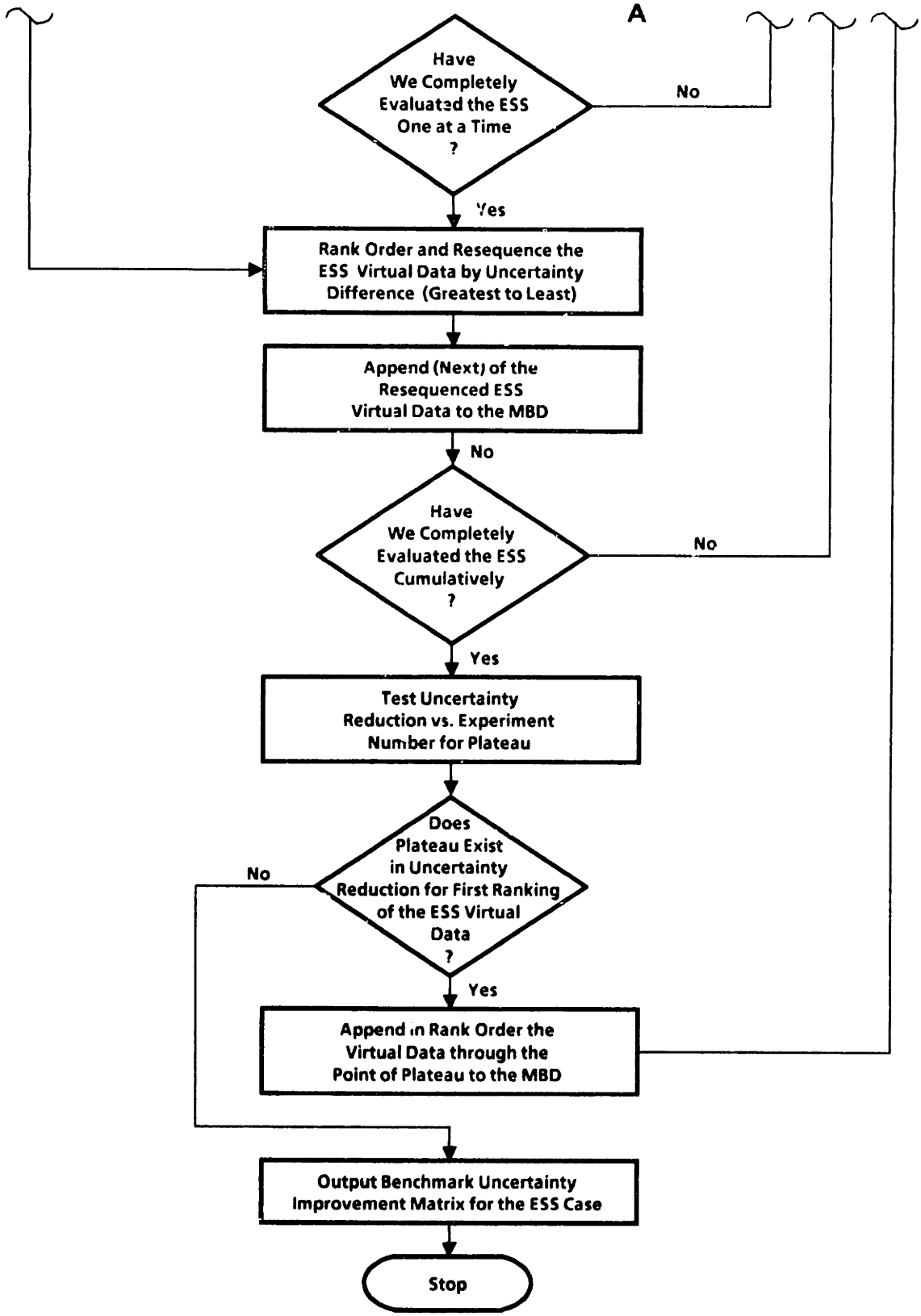
Figure 3-3 is a flowchart of the UNODEX computer program for the UNcertainty-Optimized Design of EXperiments. A source listing of the program written for this work, appears in Appendix C along with users documentation. The following sections describe the logic of the overall program and make numerous references to Figure 3-3.

3.4.1 Construction of the Experiment Sample Space

The first step in the design of uncertainty-optimized experiments is to construct the Experiment Sample Space (ESS). The ESS is a large set of candidate experiments established by restricting each of the Independent Variables (IVs) to a range such that the same mechanisms that are operating in the in-service environment will prevail. This is accomplished by reading (from a file) the preset bounds on each of the independent variables (IVs) and generating a specified number of discrete levels that the IV may assume between and including the bounding values. This is done for each of the IVs, thereby generating all combinations of IV levels. The Dependent Variable (DV) - degradation rate - is evaluated directly from the rate law using the maximum likelihood parameter estimates for each of the combinations generated and included in the ESS. These data in the ESS will be

Figure 3-3: Flowchart for Uncertainty Optimized Experiment Design




A
Have We Completely Evaluated the ESS One at a Time ?
No
Yes
Rank Order and Resequence the ESS Virtual Data by Uncertainty Difference (Greatest to Least)
Append (Next) of the Resequenced ESS Virtual Data to the MBD
No
Have We Completely Evaluated the ESS Cumulatively ?
No
Yes
Test Uncertainty Reduction vs. Experiment Number for Plateau
Does Plateau Exist in Uncertainty Reduction for First Ranking of the ESS Virtual Data ?
No
Yes
Append in Rank Order the Virtual Data through the Point of Plateau to the MBD
Output Benchmark Uncertainty Improvement Matrix for the ESS Case
Stop

referred to as 'virtual' data as they are simulated by the fitted rate law. An error must be introduced and assigned to each of the virtual data points in the ESS so as to yield meaningful uncertainty reduction estimates.

Note that the set of experiments which are generated for the ESS need not be limited to the range of expected in-service conditions if no evidence exists which indicates that exceeding that range leads to significant departure from the expected governing physical and chemical processes. Thus this methodology directly addresses the role and feasibility of accelerated life testing.

Once the ESS is generated and saved, the maximum likelihood parameter estimation algorithm is activated (just as was done to determine the parameters). This algorithm is called FITSALL and solves the P normal equations for the incremental correction to the parameter initial guesses, equations (3.20). This algorithm is dynamically dimensioned and can solve multivariable, multiparameter nonlinear functional forms provided in the function YO (the rate law). The convergence criteria are specified as a Cauchy convergence, that is the incremental change in an iteration, on the error sum of squares or on the parameters themselves. There are various other input controls which are fully documented in the appendix.

Upon determining the parameters and their errors on the initial model building pass, as was described in section 3.3 and in Figure 3-2, the parameter solution set is recorded in a file to be input as later guesses. The degradation rate law is fully specified by the function and the parameter solution set.

On the initial pass, the accumulated damage and associated uncertainty is estimated at the design life goal by the theoretical technique in 3.2.2. These serve as the reference values of damage and uncertainty for pointwise uncertainty reduction computations. They are also saved as a benchmark, or reference values for later comparison. The initial pass is complete at this point.

3.5 EXPERIMENT DESIGN: OPTIMIZATION

The second phase of UNODEX begins by "shifting" the first data point representing a candidate experiment to be entered from the ESS into the Model Building Database (MBD). In this sense data (both IV and DV) representing the first potential experiment are incorporated into the actual MBD as though actually measured. We will refer to this as simulation of an experiment and the data will be termed virtual data. Then with the MBD plus one virtual data point, the maximum likelihood parameter estimation algorithm is activated to determine updated parameters, reflecting the addition of this additional virtual data point.

The starting guesses for the parameters are the solution set which was saved in the first pass. Hence, convergence is usually rapid due to the small contribution of a single data point. The procedure is repeated for each of the virtual data in the ESS. At the end of this pointwise uncertainty estimation, the ESS is sorted and rewritten in the order of greatest to least reduction in estimated uncertainty reduction. Hence, the variable which is ranked is

$$\Delta U = \sigma_D - \sigma'_D \qquad (3.48)$$

In the above expression, σ_D is the uncertainty in penetration using the MBD only, and σ'_D is the uncertainty in penetration using the MBD + the *one* virtual data being evaluated. The final phase of the experiment design optimization is the evaluation of the uncertainty behavior at the design goal for the entire, resorted ESS. Experiments are added (without replacement) one-at-a-time from the ESS in the order determined to yield greatest to least improvement and the uncertainty reduction is calculated after each addition. This means that the final computation determines the improvement in projected uncertainty for the addition (simulation) of the first virtual experiment, then the first and second, then the first, second and third, *etc.*; until the entire ESS has been accumulated. The result of this calculation is a reduction-in-uncertainty profile dependent upon the amount of experimentation.

This type of information can allow the experimental planner to obtain an estimate of the testing requirements for a predetermined, acceptable uncertainty in accumulated damage at the design goal. The converse is also true in that an estimate of the uncertainty may be obtained for a given practical limit on experimentation.

It must be emphasized here that the above type of information must serve as a guide to experimental planning and not an absolute measure of the required number of tests, as

- The matrix employed to solve for the maximum likelihood parameter estimates was the asymptotic (infinite population) covariance matrix
- Local linearization may not be an adequate assumption, especially for poor initial parameter guesses
- Estimates of error for the virtual data may be superior to (less than) that actually obtained by measurement

3.6 SUMMARY

The previous chapter has laid the theoretical groundwork for the design of uncertainty-optimized experiments. The method is iterative and adaptive and provides a quantitative measure of an experiment's information value under the constraints and requirements of the application and in-service environment for the component under evaluation. It is a comparative method in that the asymptotic covariance matrix is used to determine the extrapolated uncertainty.

Hence, it determines the best calculable bound to the uncertainty and not an absolute measure.

The methodology has been presented in the most general sense, for any component-environment system experiencing gradual degradation in time. In the next chapter, the specifics of the particular application problem of interest, nuclear waste container life predictive testing, are introduced.

4. UNCERTAINTY-OPTIMIZED PREDICTIVE TESTING FOR A NUCLEAR WASTE CONTAINER

This chapter presents the application of the uncertainty-optimized experiment design technique to waste container penetration by general corrosion. Evaluation and assembly of the relevant data into a model building database is described, as well as the experimental methods used to obtain these data. Model development is presented, along with justification for the model's applicability and level of detail. The key task of assigning uncertainty to the virtual (or simulated) data in the experiment sample space is also discussed. Finally, a quantitative evaluation of the reduction of waste container penetration uncertainty at 300 and 1000 years is performed, yielding insight into the type and order of experiments which should be performed to reduce uncertainty most effectively.

4.1 THE EXPERIMENTAL DATA

Overwhelmingly, the body of experimental data describing the general corrosion rate of a low carbon steel in brine with compositions within the range identified in bedded halite formations has been directly commissioned by geologic nuclear waste isolation activities.

Data obtained by reviewing the technical literature have been found to be deficient in reporting the precision in principle independent variables, such as is the case pertaining to corrosion of chemical

process equipment wherein only a range of chemical conditions may be known and reported. The balance of the literature-obtained data are found to differ substantially from expected repository conditions in one or more of the independent variables.

This section serves as a review of the accessible data generated by nuclear waste disposal programs, describing the tests employed, the experimental conditions and relevance to this work.

4.1.1 Immersion General Corrosion Tests

In response to a need for standard methods to generate reliable and reproducible data measuring properties of materials used for permanent nuclear waste isolation, the US Department of Energy established the Materials Characterization Center (MCC) at Pacific Northwest Laboratory. The MCC draws upon related standard test methods such as those established by the American Society for Testing Materials (ASTM), among others. The MCC also develops new procedures and approves modifications to standard procedures where the special concerns of nuclear waste isolation require unique treatment.

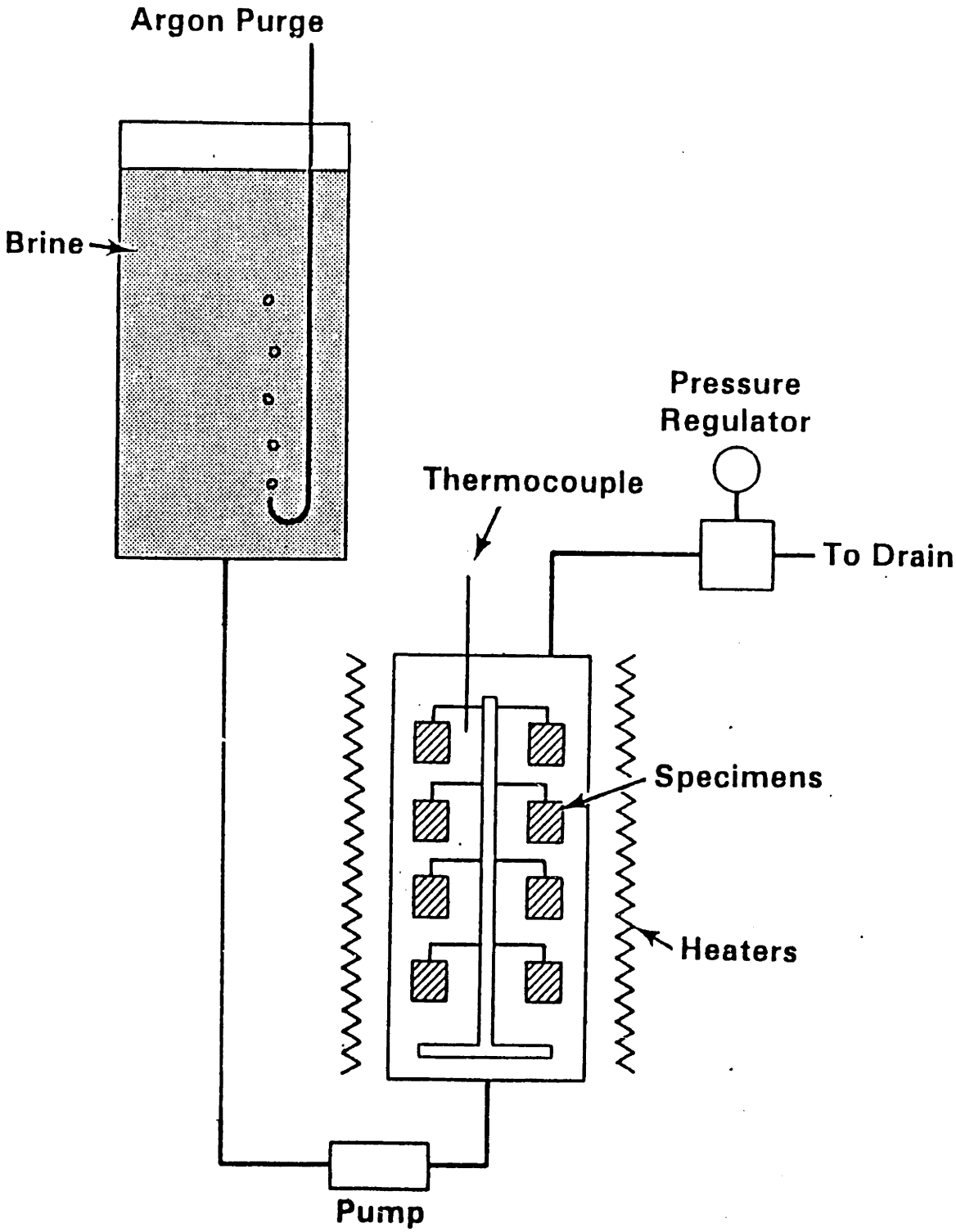
Two test methods have been developed by the MCC for evaluating both general and localized corrosion behavior of laboratory-scale specimens of waste container structural barrier materials exposed to flowing and static simulated groundwaters [36]. These tests are numbered MCC102s and MCC101s, respectively.

The autoclave system is illustrated in Figure 4-1. As indicated in the figure, corrosion specimens reside within a heated autoclave during the test. The specimens are well separated and the total surface area of specimen surface, hence, the number and size of the specimens, is determined by the autoclave volume. Brine, which is maintained anoxic by an argon purge system, is pumped through the autoclave, entering at the bottom of the vessel and exiting at the top head. Pressure and temperature are instrumented through the head.

The tests differ only in that the static immersion test allows for no solution (electrolyte) to enter or leave the autoclave during the test. The intent of the static test is to represent conditions where corrosion products are not removed from the corroding surface due to any flow mechanism. The flowing test specifies a solution refresh flow rate of roughly one vessel volume per day. The imposition of flow intends to control the electrolyte chemistry so as to be constant and to provide for the removal of corrosion products which are weakly adherent. The flowrate is not intended to simulate expected repository conditions.

The only variables which are controlled are the temperature of the autoclave and contents, and the flowrate of the solution. Both are maintained constant for the duration of the test. The other variables which could potentially affect the corrosion rate, notably the amount of dissolved oxygen and solution pH, are measured prior to the test but not

Figure 4-1: Schematic Diagram of the Immersion General Corrosion Test System



controlled. A large sealed reservoir of solution is maintained at relatively anoxic conditions by an argon purge system. The test methods specify the composition of reference electrolyte solutions which are derived from analyzed brines obtained from boreholes in the vicinity of the candidate Deaf Smith County, Texas salt repository site.

There are some slight deviations from the actual composition of the analyzed brines and those used in corrosion experiments. Permian Basin Brine 2, which was used for most of the immersion general corrosion tests, is essentially the same composition as Permian Basin Brine 1, (PBB1 in Chapter 2) with the calcium carbonate reduced by nearly 30 percent to avoid plugging of the refresh lines at the cooler points in the loop. Calcium carbonate has not been associated with a specific effect on general corrosion, hence this modification is not expected to alter the corrosion mechanisms. The balance of the test procedure is largely standard to aqueous autoclave general corrosion testing*.

Both static and flowing test methods advise investigation of various oxygen concentrations appropriate to expected barrier-repository conditions over the life of the barrier. The methods specify the ratio of test vessel capacity to total surface area of the specimen array.

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*See, for example NACE TM-01-71, Autoclave Corrosion Testing of Metals in High-Temperature Water

The corrosion data derived from such tests are entirely gravimetric in nature. Weight loss measurements are obtained after removal of corrosion products and from this direct measurement, the uniform penetration (weight loss averaged over the reacting surface) and average uniform penetration rate (uniform penetration divided by test duration) may be determined.

Microscopy and corrosion product analysis are also routinely performed at test termination.

4.1.2 Excess Salt Tests

The excess salt tests are, at the time of this writing, not documented to the level of detail of the above MCC immersion tests. Both excess salt tests were developed to evaluate the general corrosion behavior of laboratory-scale specimens of barrier materials in the presence of repository-like solid halite. The intent was to evaluate this corrosion behavior in an environment which more closely simulated the expected conditions at the waste container boundary, in which no appreciable flow conditions exist and where the corrosion product material remains in contact with the active metal, whether adherent or not, due to the presence of solid phase salt adjacent to the corroding metal. There are two basic methods of performing this type of test, in welded closed test canisters, or in an autoclave.

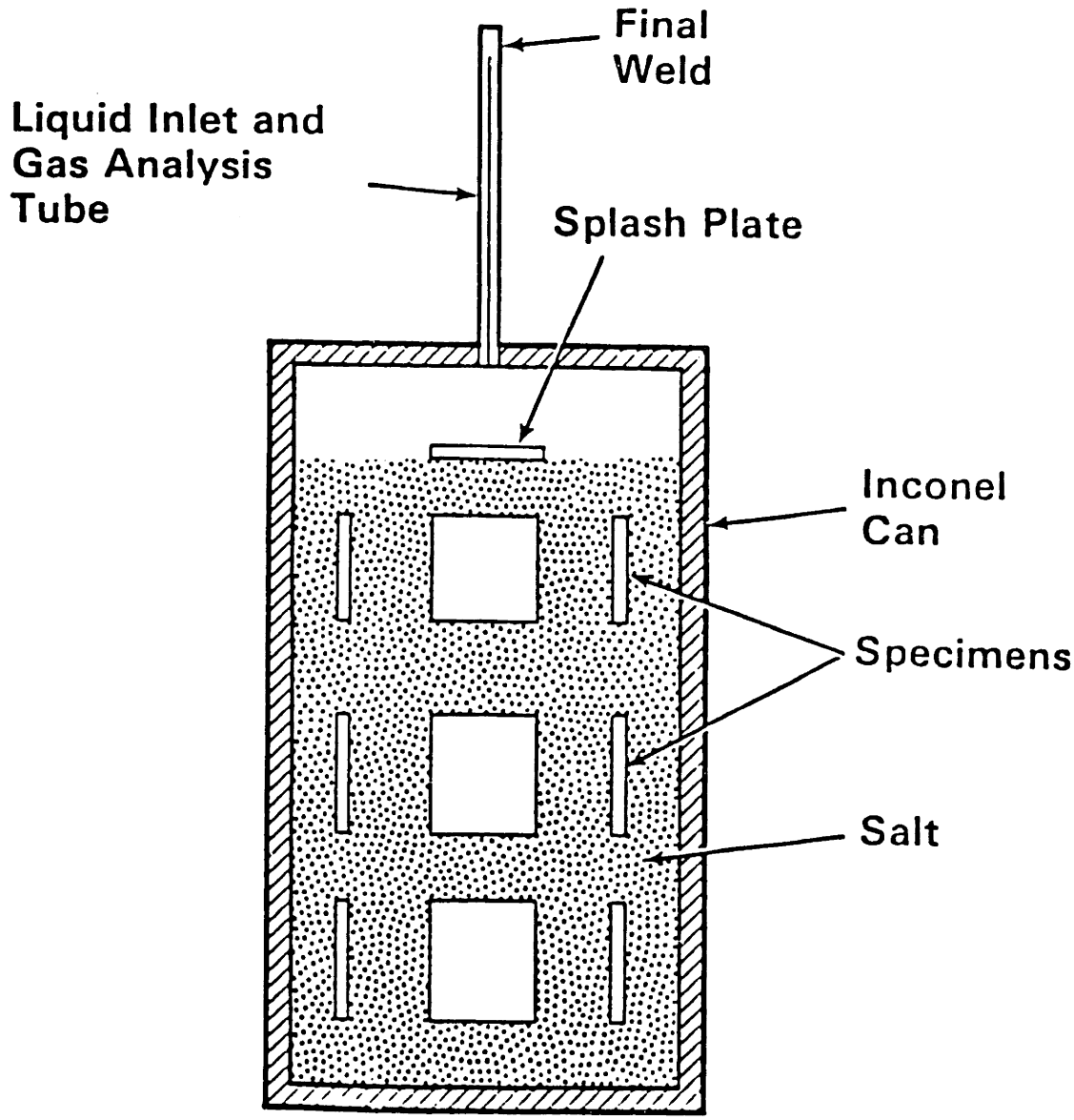
4.1.2.1 Static Excess Salt Tests

General descriptive information is available for the static excess salt tests [61] accompanying the reporting of results from such tests. The test containers are newly fabricated of Inconel 600 or other suitably corrosion-resistent material and disposed of at the conclusion of the test. The Static Excess Salt Test is represented schematically in Figure 4-2.

These containers are loaded with predried solid salt and corrosion specimens as shown in the figure. The specified moisture is arrived at by fluid addition (by either brine or water) to the dry salt-specimen array through a liquid inlet tube which penetrates the top of the cylinder. The final closure weld is performed immediately following this fluid addition under inert conditions.

The experiment is run for a fixed time-at-temperature and is, other than the temperature, uncontrolled for the duration of the test. The strength of this type of test is that it can more closely simulate the expected conditions of a waste container exposed to a predominantly anoxic, static brine environment. The weakness of this type of test is that the test may not be controlled as readily as those performed in an autoclave and has not been instrumented so as to measure control variables other than temperature.

Figure 4-2: Schematic Diagram of the Static Excess Salt Test System



This type of test is a lower cost test than the immersion tests, because there is no requirement for the use of an autoclave. Instrumenting the test is precluded by design (sealed disposable test containers) and any penetrations into the test vessel would pose a safety hazard.

The brine solution pH is measured before (at the time of preparation) and after the test termination. Dissolved oxygen content of the solution added to the salt-specimen array is known only at the time of brine preparation, however, it should be noted that the brines are maintained in anoxic conditions from the time of preparation until use.

The static excess salt test yields standard gravimetrically-derived average uniform penetration rate data and standard corrosion product information.

4.1.2.2 Autoclave Static Excess Salt Tests

This type of test was also developed at Pacific Northwest Laboratories to measure the corrosion of fully-saturated salt environments. The test is essentially the same as the Static Excess Salt Tests with the additional feature of allowing specimens to be removed and the test resumed with minimal disturbance to the balance of the corrosion specimens. The Autoclave Excess Salt Test is illustrated Schematically in Figure 4-3. This system is not pumped like the immersion tests. Small, titanium, cuplike vessels are used to hold the corrosion

specimens, packed in dried, solid phase salt much like the static excess salt tests. These specimen holders are supported by an insulated test stand within the autoclave. The autoclave is filled with brine and maintained at pressure and temperature for the entire test.

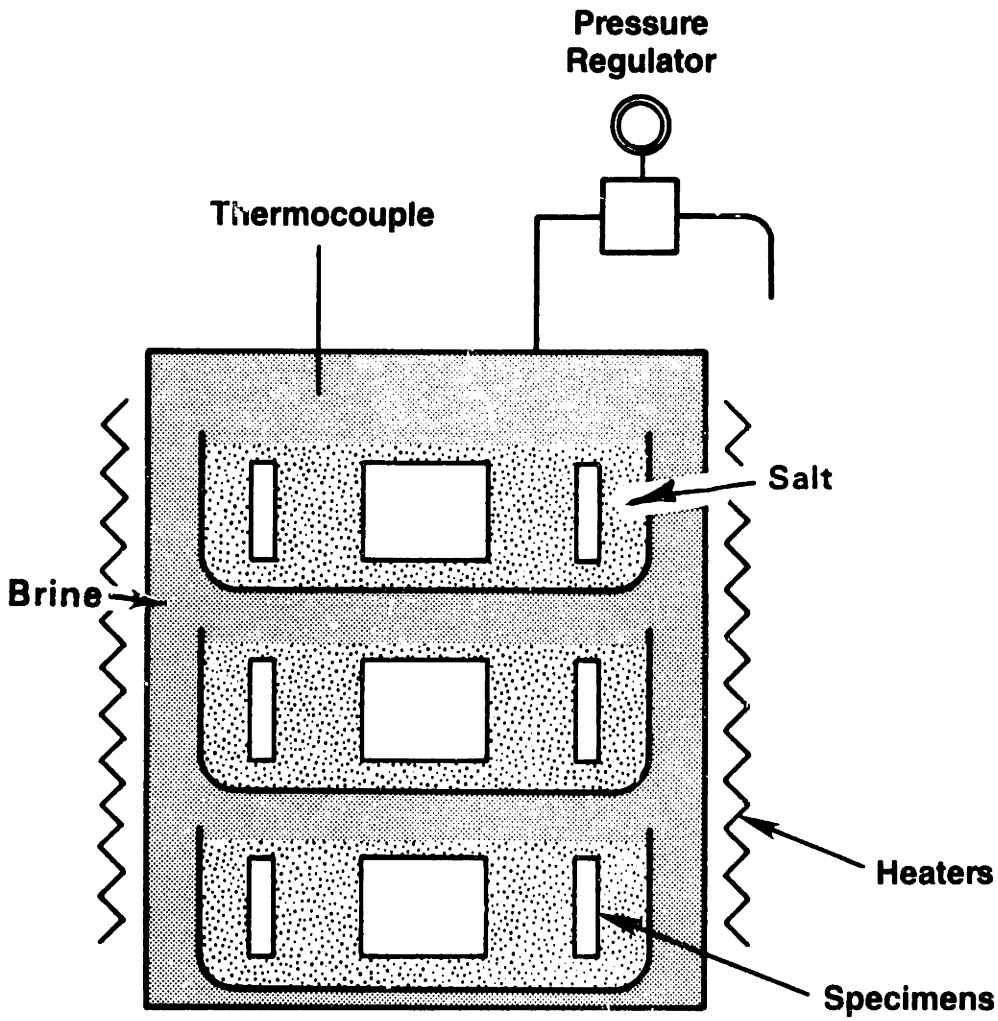
4.1.3 Assembly of the Database

With the intended purpose of developing a multivariable model of waste container alloy corrosion in the relevant environment by maximum likelihood parameter estimation, data generated via the experimental methods described above were assembled into a large database. These data were grouped together although they were obtained by different test methods. This grouping was necessary in order to obtain a sample possessing a significant range in each of the independent variables common to the measurements. The independent variables common to all tests and deemed potentially the most significant to the corrosion system under study (see model development section below) are:

- Temperature
- Dissolved Oxygen Concentration
- Magnesium Concentration
- Total Fraction of Water in the Test
- Time

The selected dependent variable is the average uniform penetration rate (henceforth called the corrosion rate).

Figure 4-3: Schematic Diagram of the Autoclave Excess Salt Test System



Some explanation follows regarding the above independent variables. Temperature was always held constant and reported for every measured corrosion rate. With the exception of only one series immersion general corrosion tests, the dissolved oxygen was controlled to - or was presumed to be - near the limits of control, as all brines were prepared or maintained under an argon purge system. This limit of control for brine at anoxic conditions for the experimental programs described above has been reported to be 0.05 ppm.

In all cases, the magnesium concentration was calculated from brine compositions particular to the test, and the ratio of brine to salt mass. Mass-average magnesium concentrations were calculated for all excess salt tests, and the brine solution magnesium concentration was used for the immersion tests.

The following three tables, 4-1, 4-2 and 4-3, display the conditions for which data were included in the corrosion database, later to be used to generate maximum likelihood estimates of the multivariable model parameters. The computer data file is included in an appendix to this thesis.

Table 4-1: Test Conditions Summary for Data Generated by Immersion General Corrosion Tests

Temperature (C)	Oxygen (ppm)	Magnesium w/f	Water w/o	Time (hrs)	Number (reps)
90	0.05	0.0465	76	745-4424	(6)
150	1.50	0.0001	76	736-5384	(13)
150	0.05	0.0001	76	336-5635	(30)
150	0.05	0.0468	76	144-4924	(12)
150	0.05	0.0009	76	677- 773	(4)

Table 4-2: Test Conditions Summary for Data Generated by Static Excess Salt Corrosion Tests

Temperature (C)	Oxygen (ppm)	Magnesium w/f	Water w/o	Time (hrs)	Number (reps)
90	0.05	0.0001	5	2155-2198	(3)
90	0.05	0.0001	20	2155	(3)
90	0.05	0.0034	5	2155	(3)
90	0.05	0.0134	5	2203	(6)
150	0.05	0.0001	5	2155	(3)
150	0.05	0.0001	20	2155-2198	(9)
150	0.05	0.0004	20	759	(4)
150	0.05	0.0034	5	2155	(3)
150	0.05	0.0042	5	2178	(6)
150	0.05	0.0081	10	2178	(6)
150	0.05	0.0134	20	2179	(3)
150	0.05	0.0170	20	767-2178	(12)
150	0.05	0.0220	25	2178-7031	(12)
150	0.05	0.0270	30	1659-2178	(12)
200	0.05	0.0001	5	2155	(3)
200	0.05	0.0034	5	2155	(5)

Table 4-3: Test Conditions Summary for Data Generated by Autoclave Excess Salt Corrosion Tests

Temperature (C)	Oxygen (ppm)	Magnesium w/f	Water w/o	Time (hrs)	Number (reps)
150	0.05	0.0468	76	762-2181	(4)
150	0.05	0.0353	53	672-2124	(8)

4.2 DEVELOPMENT OF A MULTIVARIABLE MODEL FOR GENERAL CORROSION

To date, there have been no published attempts to describe the fate of waste container alloys by uniform dissolution (or any other mechanism of slow degradation) in repository-relevant environments. This is largely due to the complexity of the geochemistry of brines expected at the repository horizon, and the uncertainty in the amount and mechanism of transport of these brines to the container surface. More mechanistic models will undoubtedly become available as onsite in-situ testing proceeds. Some simple correlations have been developed based on small samples of laboratory experiments, often called screening or scoping tests. These test are usually performed to evaluate various alloys comparatively, rather than for the purpose of investigating the mechanisms underlying corrosion in the system.

What is required for an analysis of waste container degradation - and more importantly - its associated uncertainty, is a multivariable model of the general corrosion rate. The model should include the most significant variables understood to affect this rate. Also, projected time dependent behavior for all of these significant variables must be estimated, which will allow the computation of time- and environment-integrated penetration.

This section describes the model which has been developed as a first attempt at modeling the most significant of the variables - in

combination - shown to effect the general corrosion rate of the A216 low carbon steel in repository-relevant environments.

4.2.1 Determination of the Principle Variables

4.2.1.1 Temperature

Temperature at the waste container - salt brine interface will increase slightly to a maximum at approximately five years. The temperature will be ever-decreasing after that time (See Figure 2-4).

The system considered, a low carbon steel in neutral pH aqueous environment has been shown to exhibit ever decreasing but continuous corrosion behavior. This indicates that the overall corrosion product formed at the surface of the metal never provides a solution-impermeable passive film. The film which forms at these conditions acts to retard solution access to the active corroding surface.

Fluid transport through this film may be accomplished either by repeated formation-and-rupture with a gradual accumulation of non-adherent corrosion products surrounding the actively forming layer, or by the continuous formation of corrosion products (such as amakinite) which are permeable to aqueous solutions.

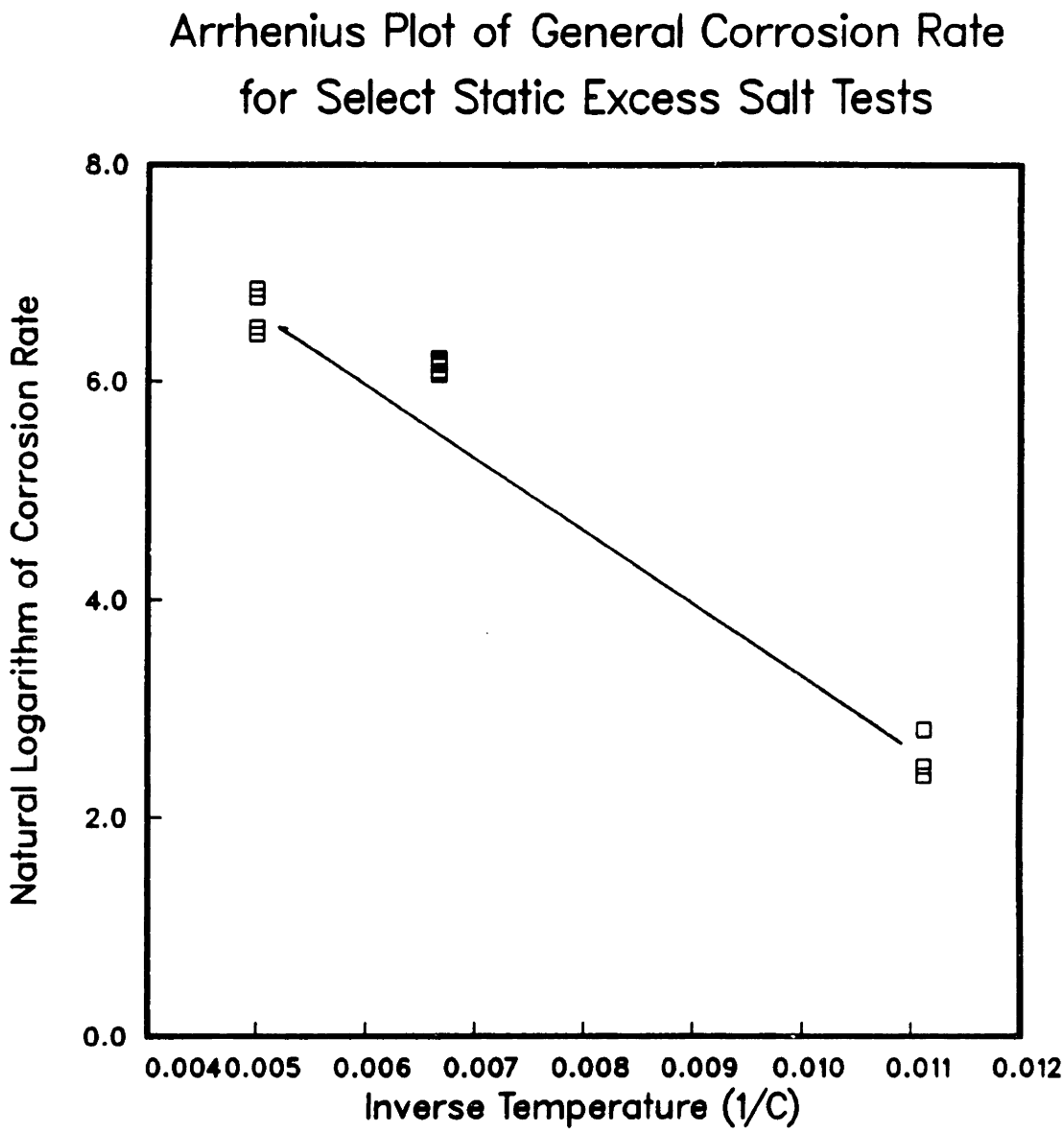
These types of chemical processes, which involve solution diffusion through a thickening corrosion product barrier and multiple reaction steps, may be thought of as having an apparent overall activation energy associated with the charge transfer step.

The sparse, compatible data at differing temperatures is presented in Figure 4-3 below. This plot presents the natural logarithm of the corrosion rate of the A216 alloy as a function of inverse test temperature in Figure 4-3. This type of plot is often called an Arrhenius plot; and the linear slope obtained from the curve is an estimate of the (constant) activation energy. Linearity implies a constant activation energy for a single physical degradation mechanism. Regarding the data at 150°C, these measurements are actually generated by an environment of higher magnesium concentration, 0.0042 as opposed to 0.0034. It will be discussed below that increased magnesium concentrations are shown to increase the corrosion rates nonlinearly. Accounting for the greater corrosion rate for the 150°C data might provide even more confidence in the linearity of the Arrhenius plot. The other test conditions were: anoxic (approximately 0.05 ppm), 5 weight percent water and a test duration approximately 2200 hours.

Based upon the line drawn in Figure 4-3, which, from the discussion above indicating the reasons for the higher corrosion rate at 0.0067, is essentially fitted to the endpoint data, the resulting activation energy is 13.32 kcal/mole.

The temperature at which the chemical reaction takes place will also determine what thermodynamically-stable corrosion products will form, the solubilities of chemical components in the brine, and potentially the arrival rate of thermomigrating brine.

Figure 4-4: Temperature Dependence of the Corrosion Rate



4.2.1.2 Dissolved Oxygen

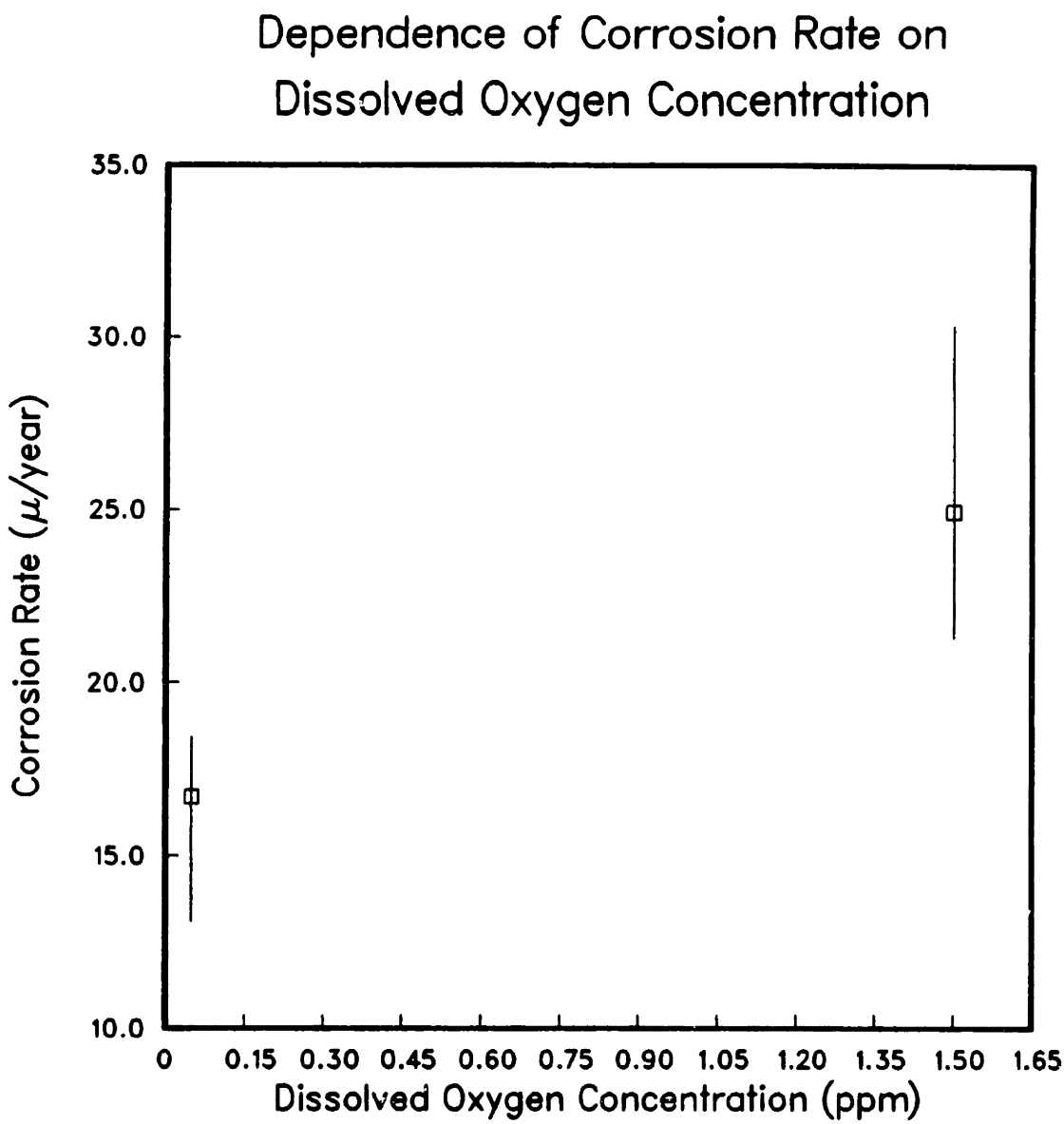
Compatible data for immersion general corrosion tests conducted at anoxic (approximately 0.05 ppm) and oxic (approximately 1.50 ppm) conditions are presented in Figure 4-4. The vertical bars through the data represent actual measurement spread (bounded by the maximum and minimum observed rates) and the plotted points are the mean of the measurements.

Clearly the oxygen-rich environment provides for more rapid dissolution of the metal. The increased oxygen level raises the system Eh (oxidation potential). It has been shown in Figure 2-8 the polarization behavior of A216 steel in magnesium-rich brines indicates the increase of corrosion rate (current) with Eh.

4.2.1.3 Magnesium Concentration

The results of polarization resistance measurements for A216 steel in electrolytes varying in magnesium ion concentration are excerpted from Golis [26] and presented in Figure 4-6. Data which are displayed as corrosion rate are actually inferred from measurements of resistance at the corroding metal surface. With a known electric potential, and the measured resistance, the corrosion current may be calculated. It has been noted previously (Chapter 2) that low carbon steels in highly concentrated magnesium brines exhibit greater corrosion rates, hence the importance of this variable in repository-relevant environments will not

Figure 4-5: Dissolved Oxygen Dependence of the Corrosion Rate



be further justified here. These electrochemically determined results appear to indicate a nonlinear, monotonic increase in general corrosion rates with magnesium concentration and further confirm the absence of any passivation behavior.

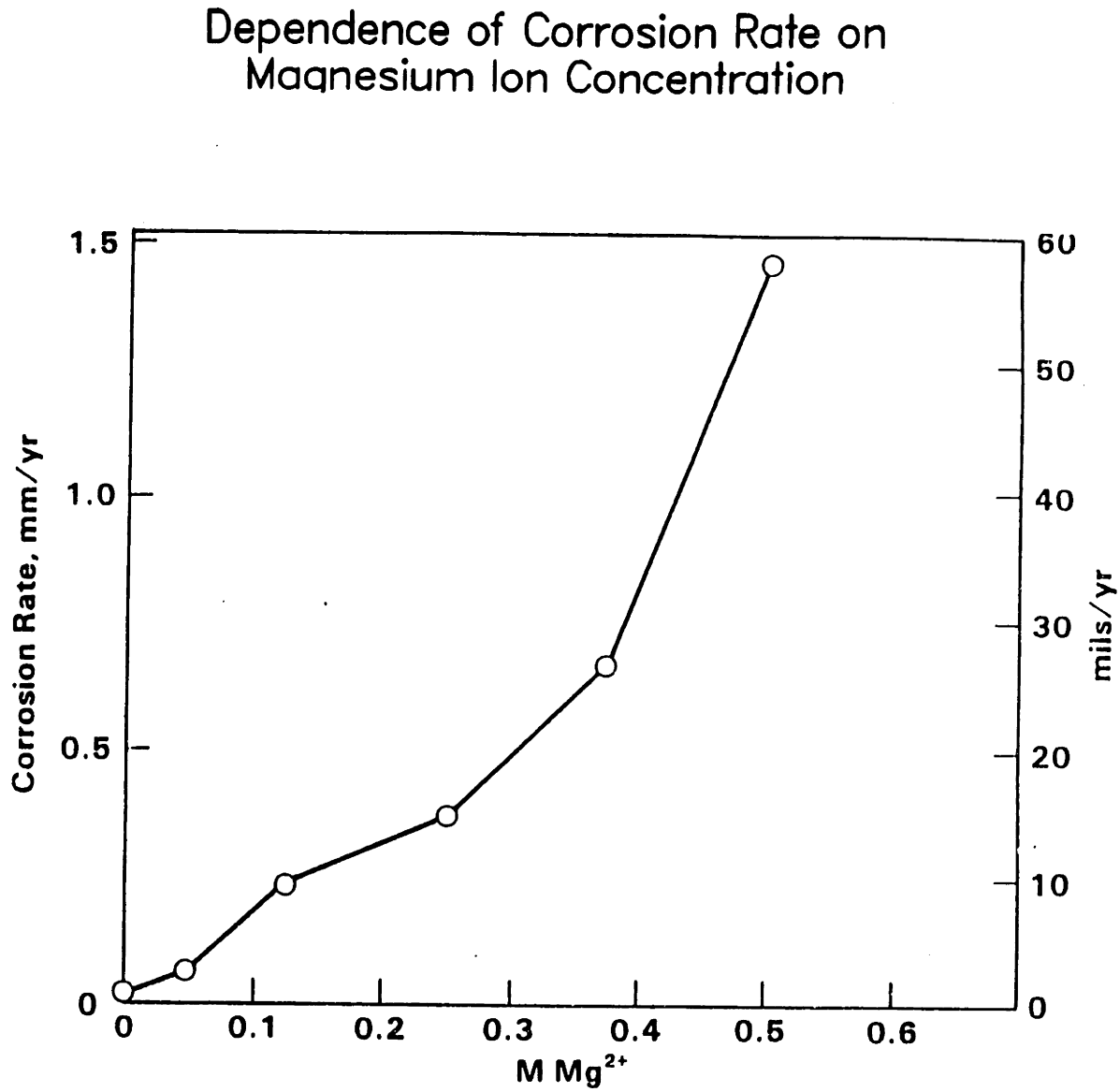
4.2.1.4 Total Fraction of Water in the Test

The variable referred to as 'total fraction of water in the test' attempts to represent the condition of dryness of the interfacial corroding environment. As has been discussed in Chapter 2, the bedded halite and mudstone host rock at the repository horizon are quite plastic and are suspected of flowing so as to contact the waste container surface in a relatively short time, (order of 1 year). The average moisture content of the halite and mudstone is approximately 1.64 weight percent. Based on this consideration it is assumed that the interfacial corroding environment may be represented by a time-dependent boundary condition of solid/liquid phase salt/brine throughout its life in service.

Data have been obtained for general corrosion in conditions from 5 weight percent water and the balance solid salt in a static excess salt test to all brine immersion tests which are 76 weight percent water, the balance being dissolved solids, predominantly sodium chloride.

The results of Westerman, et. al. taken from Golis [26] are presented for consistent static excess salt measurements conducted at 150°C, in

Figure 4-6: Corrosion Rate Dependence on Magnesium Concentration from [26]



PBB1 salt/PBB3 brine in Figure 4-6. The tests were conducted for three months. The general trend in these results indicate an increasing corrosion rate with greater water fractions.

4.2.1.5 Time

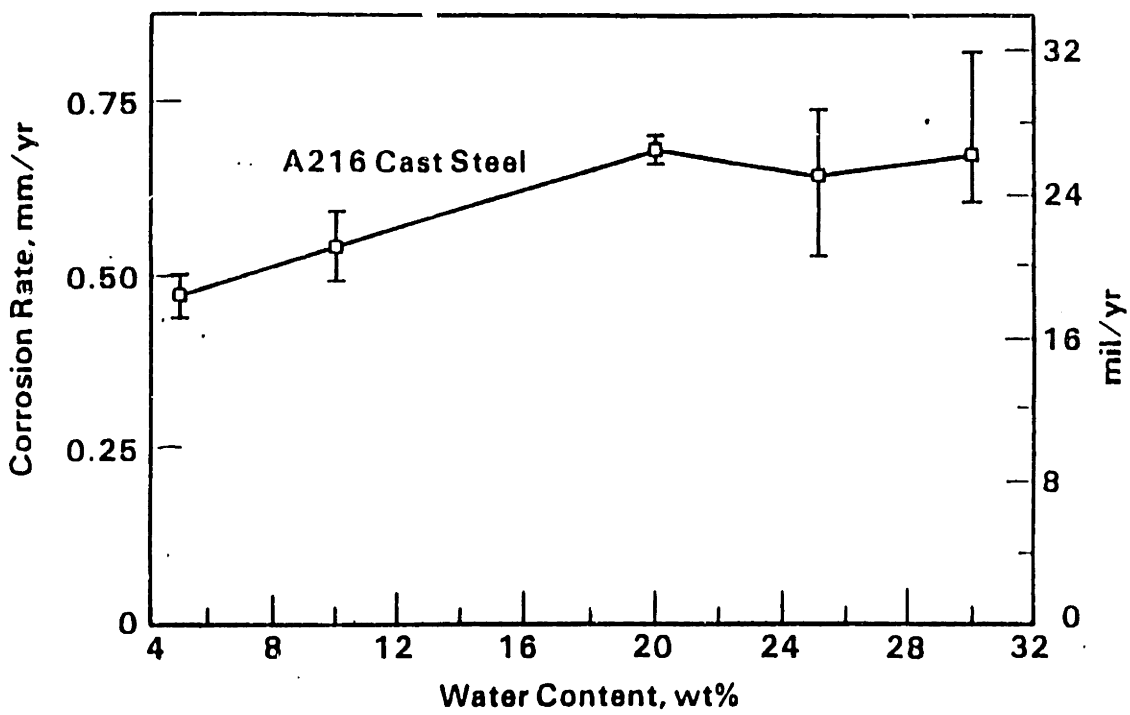
Finally, time is of course one of the principle variables affecting the general corrosion rate. Gross oxidation behavior of metals is most often investigated by measuring and empirically correlating the rate of oxidation (via weight loss measurements) with time. Rate constants are obtained in this way. Wagner [22] showed theoretically that a pure metal would obey a parabolic oxidation rate law, given that the oxidation rate was controlled by ionic diffusion through a continuously thickening oxide layer. This corrosion rate, y, is given by:

$$y = k\,t^{-1/2} \qquad (4.1)$$

The parameter k is called the parabolic rate constant.

It should be pointed out that this behavior is derived for an ideal metal experiencing dissolution by a single oxidizer. Deviations of actual measurements to exhibit parabolic corrosion rate behavior often only indicate the presence of morphological inhomogenieties [22] at the reacting metal surface and the developing oxide film. Time raised to other fractional powers are often correlated with empirical measurements to correct for this non-ideal behavior.

Figure 4-7: Water Content Dependence of the Corrosion Rate from [26]



Peters and Kuhn [46] have developed a correlation for a limited number of high-magnesium brine static excess salt tests. Their model assumes that the corrosion penetration was proportional to the magnesium ion concentration at the reacting metal surface. The resulting general functional form for the penetration rate, y, is

$$y = (A + B\,t)^{-1/2} \qquad (4.2)$$

where A and B are fitted parameters. The time dependent penetration resulting from this model (from Golis [26]) is depicted in Figure 4-8.

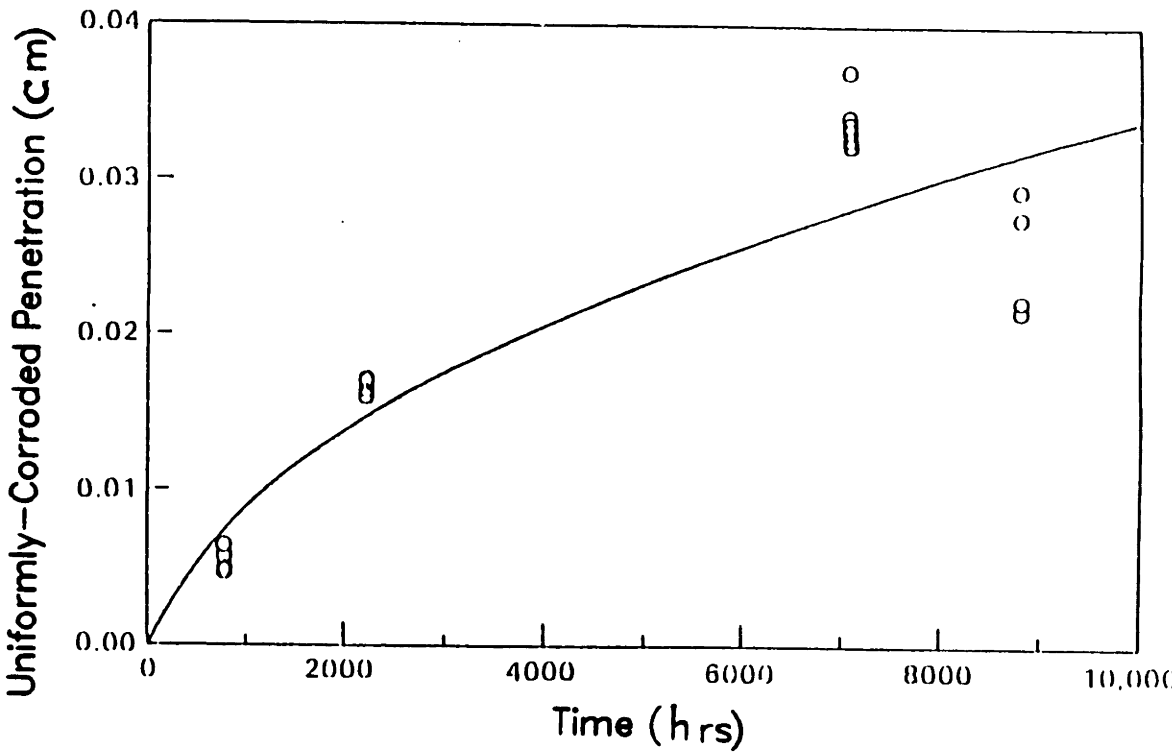
4.2.2 Comparison of Models Considered

It may be concluded from the above information that the corrosion rate of A216 steel in repository like environments will corrode at a rate which:

- Increases with increasing dissolved oxygen concentration, magnesium concentration and total fraction of water at the reacting surface.
- Is controlled by less-than-linear kinetics, hence the gross time dependent behavior will depend on some reciprocal fractional power of time.
- Exhibits an apparent Arrhenius activation energy for the overall reaction process, hence may be cast in an overall Arrhenius formulation.

Table 4-4 presents the functional forms of the alternative models which were evaluated with the data set. A brief explanation of each model is included in the table. Also tabulated for the alternative

Figure 4-8: Uniform Penetration Time Dependence from [26]



models is the (unbiased) sum of the squared errors. This measure serves as a simple comparative criterion for goodness of fit which characterizes each of the equations. The models which include a polynominal time term exponentiated by a parameter diverged with even small changes made to this exponent parameter. Fixing the parameter at a constant value of 1/2 improved the convergence and fit considerably, as in model number 3 of the table. In the fitting of model 3, the maximum likelihood estimates determined did not result in any lower error sum of squares than the initial guess values. The fourth model, a steady state case, represented an attempt to investigate the need to include an explicit time- dependent term. This steady state functional form was abandoned, also due to lack of convergence. The fifth model, a modified Eyring Model, was chosen as the best among the alternatives. In this model the activation energy, parameter b_6, is reduced by a magnitude which is a linear function of the other three corrosion-accelerating variables; dissolved oxygen, magnesium concentration and total water fraction. This model has associated with it the lowest error sum-of-squares deviation which is achievable by any of the listed forms. The kinetic prefactor is also somewhat modified from Wagner's theoretical parabolic rate behavior, but can be forced to behave similarly depending upon the values of b_1 and b_2.

Table 4-4: Corrosion Rate Models Considered

Model	Sum of Squares
$\frac{b_1}{(b_2+t)^{b_3}} \exp\ b_4 x[O] + b_5 x[Mg] + b_6 x[H_2O]\ \exp \frac{-b_7}{T}$	$1.597*10^7$
$\frac{b_1}{(b_2+t)^{b}}\ b_4 x[O] + b_5 x[Mg] + b_6 x[H_2O]\ \exp \frac{-b_7}{T}$	$1.248*10^7$
$\frac{b_1}{(b_2+t)^{1/2}}\ b_4 x[O] + b_5 x[Mg] + b_6 x[H_2O]\ \exp \frac{-b_7}{T}$	$2.324*10^7$
$b_1\ b_4 x[O] + b_5 x[Mg] + b_6 x[H_2O]\ \exp \frac{-b_7}{T}$	$1.059*10^7$
$\frac{b_1}{(b_2+\sqrt{t})^{b}} \exp\ b_4 x[O] + b_5 x[Mg] + b_6 x[H_2O]\ \exp \frac{-b_7}{T}$	$8.732*10^6$

Where:

t	=	Time (hours)
[O]	=	Dissolved Oxygen
[Mg]	=	Magnesium Concentration
$[H_2O]$	=	Water Fraction
T	=	Temprature (°C)

4.2.3 Results of the Model

In order to predict the general corrosion penetration and uncertainty with the above model, the expected in-service environment must be specified for a time period extending to the desired design life of interest. This specification may take the form of known time varying values for the independent variables included in the model.

4.2.3.1 Specification of the In-Service Environment

Results were obtained from the TEMP* code for the temperature profile at the waste container surface as a function of time. The reference package design parameters of Table 2-1 were used in these calculations for a horizontally emplaced waste package. The other five variables, for lack of better assumptions, were held constant over the 1,000-year time projection. Table 4-5 lists the timesteps and the assumed value of the variable (held constant) in that timestep. These values will become the reference case for the time dependent environmental boundary conditions at the corroding metal surface. These conditions will be used as arguments to the corrosion rate law and to determine the time-integrated penetration. A limited number of variations in this assumption will be analyzed below.

Repeated fits of the data with various initial starting guesses indicated that the parameter for the constant activation energy, b_6,

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*Wurm, *et. al.*, see reference [65]

Table 4-5: Assumed In-Service Environmental Independent Variables

Temperature (°C)	Dissolved Oxygen (ppm)	Magnesium Concentration (w/f)	Water Fraction (w/f)	Time (years)
134.6	0.05	0.05	0.05	1.0
134.9	0.05	0.05	0.05	2.0
134.4	0.05	0.05	0.05	5.0
130.7	0.05	0.05	0.05	10.0
124.5	0.05	0.05	0.05	20.0
106.7	0.05	0.05	0.05	50.0
89.4	0.05	0.05	0.05	100.0
75.3	0.05	0.05	0.05	200.0
72.0	0.05	0.05	0.05	300.0
66.1	0.05	0.05	0.05	500.0
59.9	0.05	0.05	0.05	1000.0

generally converged near the same constant value for minimum sum of square error. It was decided, based on the nearly always constant value obtained, 5793 (^{o}C), to fix this parameter as a constant term at that value. This is physically consistent with the assumption that the apparent activation energy of the overall corrosion mechanism remains constant all but the variables oxygen, magnesium and water fraction which are explicitly included. This leads to a constant activation energy of 11.51 kcal/mole, which compares well to the estimated value of 13.32 kcal/mole arrived at from the simple Arrhenius plot, Figure 4-3.

In a similar way, the parameters for dissolved oxygen and water fraction were found to only weakly influence the overall fitting process. They were assigned the constant values which were obtained on the converged fit yielding the sum of square error value tabulated. All of the maximum likelihood estimate parameter values are presented in Table 4-6. These values were determined by the maximum likelihood estimation technique of Section 3.2.2, Equations (3.22), (3.31) and (3.33), codified in the FITSALL algorithm (a subroutine of the UNODEX Program in appendix). Relevant computational constraints on the problem are also presented in the table.

A scheme for weighting the ESS virtual data which is also used to weight the MBD is discussed in Section 4.3.1.1 below and will not be presented here. However, the following penetration and uncertainty results have been calculated employing this weighting scheme.

Table 4-6: Maximum Likelihood Parameter Estimates for the Corrosion Rate Model

TERMINATION CONDITION	NEGLIGIBLE CHANGE IN SUM OF SQUARES
NUMBER OF ITERATIONS	4
B_1	1.2782757E+11
B_2	7.8842731E+02
B_3	1.6418113E+04
ERROR SUM OF SQUARES	8.75412E+06
VARIANCE	4.89057E+04
SAMPLE STANDARD DEVIATION	2.21146E+02
AVERAGE DEVIATION	6.17274E+00
AVERAGE RELATIVE DEVIATION	-3.73631E+00

The multivariable model of general corrosion displayed as Table 4-4, number 5 becomes:

$$y = \frac{1.29*10^{11}}{774.5\#+\#\sqrt{t}} \exp 0.088[O] + 1.39x10^{-8}[H_2O] + 1.62x10^{4}[Mg] - \frac{5793}{T}$$

using the fitted parameters of Table 4-6 where y is the penetration rate in μ/year, t is in hours and T in °C.

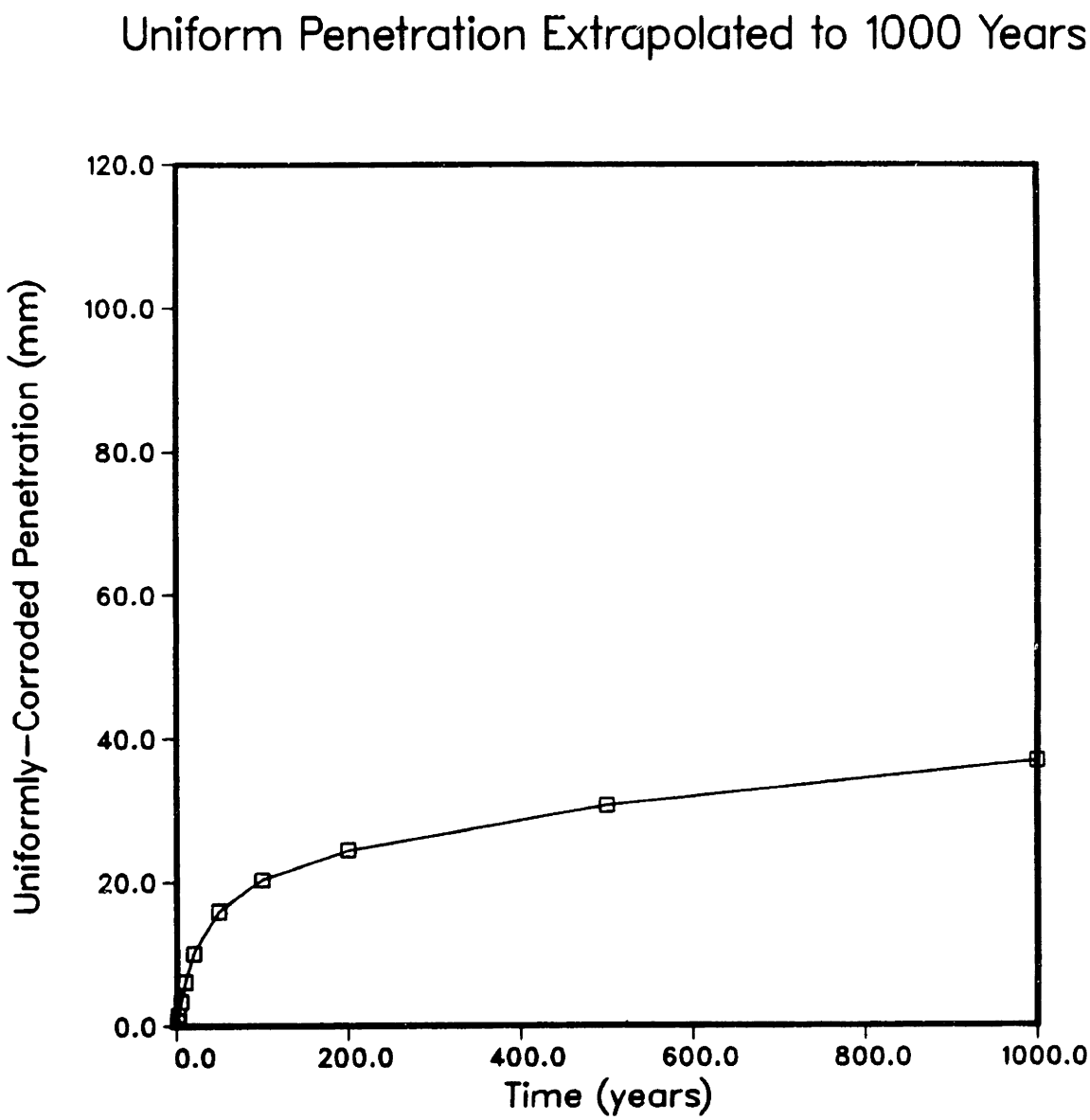
We make the following explicit approximations and assumptions allowing the numerical evaluation of environment-dependent penetration and uncertainty:

- The fitted constants (parameters) of the corrosion rate model and their uncertainty in a given time interval are independent from the other time intervals (Note the corrosion rate *is* time-dependent).
- All the influential environmental independent variables are represented in the rate law model.
- The functional form of the rate model is correct.
- The environmental independent variables may be approximated by constant values within each given time interval.
- The mechanism which produced the measured values in the Model Building Database, which was used to generate the MLE parameters, prevails over the independent variable space defined by the specified in-service environment.

4.2.3.2 Analysis of Waste Container Penetration and Uncertainty

Given the multivariable model of general corrosion, the specified in-service environment and the assumptions above, the resultant penetration in time behavior is fully determined and presented in Figure 4-9.

Figure 4-9: General Corrosion Container Penetration
Reference in-service boundary conditions: Temperature profile as given in Table 4-5, O:0.05 ppm, Mg:0.05 w/o, W:0.05 w/f



This exhibited behavior possesses the salient feature of an ever declining corrosion rate, hence the time-integrated penetration slowly approaches an asymptotic value. If the 10,000 year value is selected for the asymptote* this computed asymptotic value is 5.80 cm, hence the penetration only doubles the 1000 year value in the subsequent 9000 years.

Based on a total penetrated thickness of the container after the 1000 year interval of 2.93 cm, a corrosion allowance concept is quite acceptable. However, the more significant design parameter when considering very long term containment is the uncertainty in the above penetration. Based on the propagation of the random errors, described by Equations (3.43) - (3.46), the uncertainty in 2.93 cm at 1000 years is 2.11 cm, or 72% of the total. This uncertainty is assessed on the random error about the measured data and does not incorporate any uncertainty due to environmental boundary condition variations (*e.g.* arrival rate of brine) spatially nonuniform attack or other fundamental nonuniformities in general corrosion process (*e.g.* lack of homogeniety in the container itself). The reference penetration and 2σ confidence interval are presented as Figure 4-10. The computed lower confidence bound was constrained by an assumed irreversibility condition. The

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*Most of the federal regulations and design constraints on the engineered barrier system end after this interval.

penetration along this bounding limit was never allowed to decrease, as metal deposition is not expected to be a viable mechanism for thickening of the container wall. This bound was fixed at its maximum value in time, once obtained, of 2.27 mm, at 10 years.

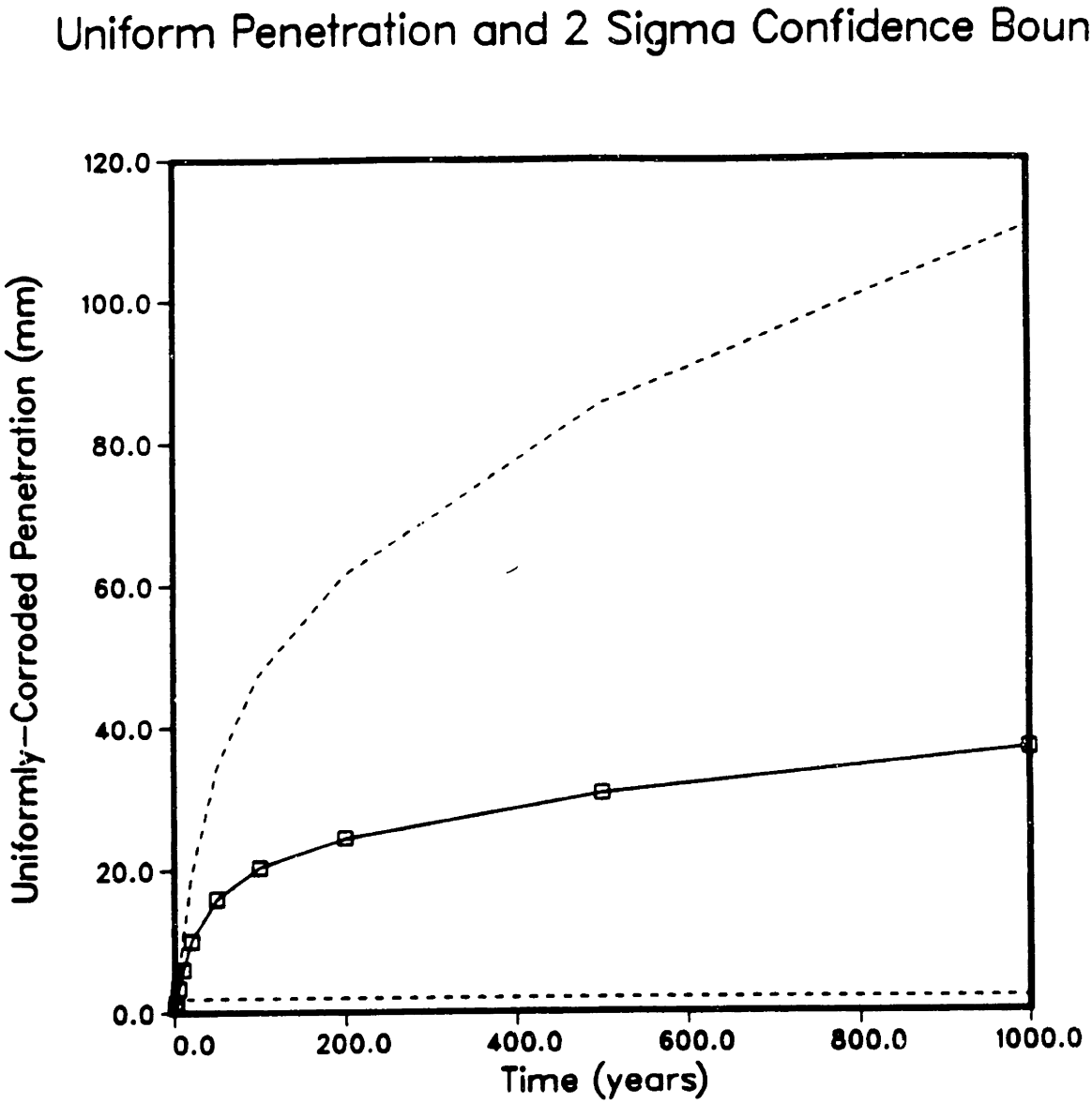
The reference conditions assumed for the cases illustrated in the above Figures 4-9 and 4-10 were calculated based upon relatively 'conservative' in-service environmental boundary conditions. Specifically the physical statements of these assumptions are

- There is infinite reserve of high-magnesium brine available via some means of transport to the container boundary.
- The rate of this brine availability is never the limiting step in the overall process of metal dissolution.
- The dissolved oxygen concentration in the brine is always anoxic (0.05 ppm)
- The container-salt interface is always characterized by 5 weight percent water (by brine) and 95 weight percent solid phase salt.

Due to the lack of knowledge regarding the above assumed environment, some limiting cases varying the assumed in-service environmental boundary conditions are commonly made and sensitivity of the results to these changes are determined.

The source of highly concentrated magnesium brine in halite formations such as in the Palo Duro Basin are the intracrystalline brine inclusions discussed in Section 2.3.2. These fluid inclusions are proposed to

Figure 4-10: General Corrosion Container Penetration and Uncertainty Reference in-service boundary conditions: Temperature profile as given in Table 4-5, O:0.05 ppm, Mg:0.05 w/o, W:0.05 w/f



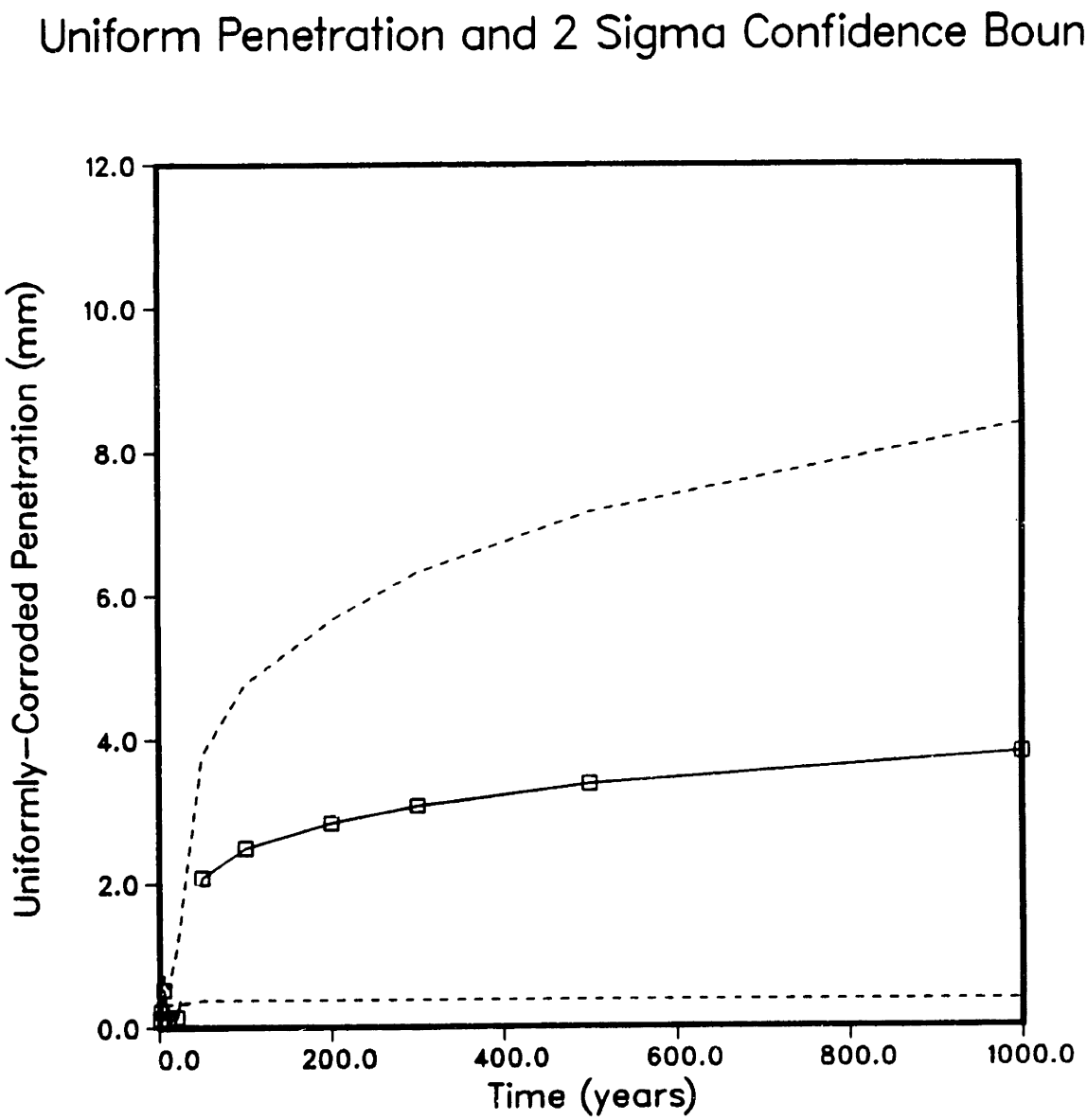
migrate to the container surface due to thermal gradient-driven transport. The intercrystalline brine and brines resulting from water intrusion (by some unspecified mechanism) and subsequent dissolution of host rock salt are quite low in magnesium concentration, however. Hence it is useful to postulate that the relevant chemistry is that of a low magnesium brine which reflects both the water intrusion scenario and the mixing of intra- and intercrystalline brines before reaching the container interface.

With all environmental conditions held the same as for the reference case except the magnesium concentration, which was fixed at 0.005 ppm, the results of Figure 4-11 are obtained.

The sensitivity of the corrosion rate to magnesium concentration is obvious from the results presented in Figure 4-11. Based on the low magnesium case, the total penetration after 1000 years is 3.81 mm with a standard error of 2.29 mm. The 2σ confidence interval would yield a worst anticipated penetration of 8.39 mm.

In order to assess the scenario of limited brine availability, which may be justified on the bases of the theory of the existence of a thermal gradient 'cutoff' value for thermomigrating brine inclusions, the corrosion rate of the above model was fixed arbitrarily small after 200 years to 1 micron/year. The cutoff time was derived from the brine

Figure 4-11: General Corrosion Penetration and Uncertainty for Low Magnesium Brine Reference in-service boundary conditions: Temperature profile as given in Table 4-5, O:0.05 ppm, Mg:0.05 w/o, W:0.005 w/f



accumulation calculations published in the Final Environmental Assessment for the Deaf Smith County Texas site, USDOE [55]. Results of the Deaf Smith Environmental Assessment indicate, with a thermal gradient cutoff of 0.125 ^{o}C/cm, that the total volume of accumulated brine per package essentially reaches its asymptotic value of 0.83 m^3 at 200 years. The computations are based on the Jenks Equation (2.1).

The results of the corrosion rate cutoff at 200 years are presented in Figure 4-12 below. As can be observed in the figure, the uncertainty after the cutoff increases only slightly as changes in variance coefficients (Equation (3.43)) only alter the uncertainty in an infinitesimal rate, leading to a very small time-integrated change in accumulated penetration.

One final case in varying the in-service environmental conditions is necessary, that of the temperature profile. This is important to computations of container penetration for the reference commercial high level waste loading, which has a greater power output in the early years due to the higher loading of 9.5 kW/package (compare Table 2-1). The temperatures employed for this waste container loading were obtained from results published in the Final Environmental Assessment for the Deaf Smith County Texas site, USDOE [55] and are tabulated in Table 4-7. As is demonstrated in Figure 4-13, according to the model of general corrosion developed above, higher temperatures result in much more rapid

Figure 4-12: General Corrosion Penetration and Uncertainty Incorporating Brine Availability Cutoff at 200 Years Reference in-service boundary conditions: Temperature profile as given in Table 4-5, O:0.05 ppm, Mg:0.05 w/o, W:0.05 w/f up to 200 years

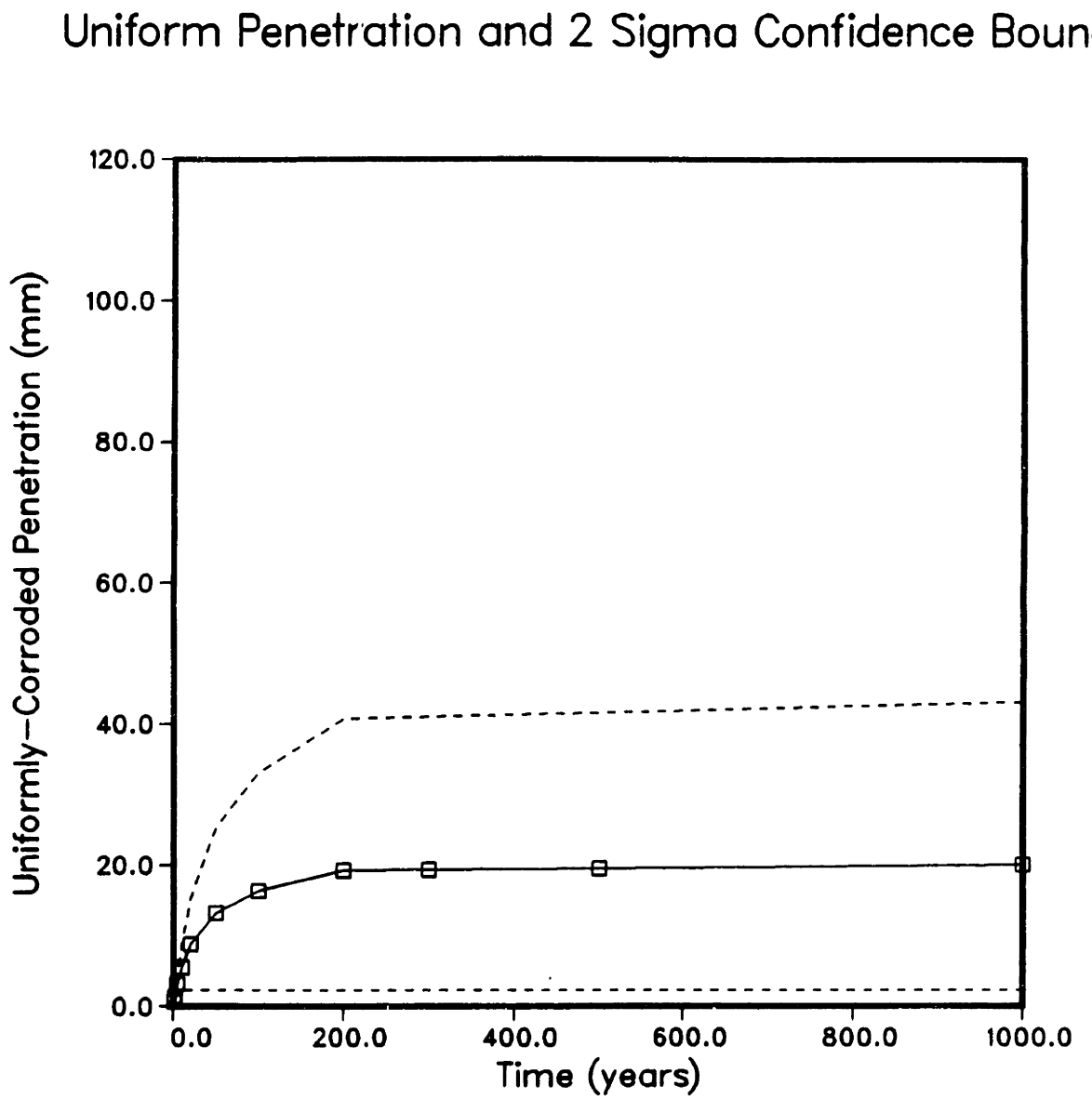


Table 4-7: Container Boundary Temperatures for the Commercial High Level Waste Loading, 9.5 kW

Time (years)	Temperature (°C)
1.0	212.0
2.0	220.0
5.0	227.0
10.0	225.0
20.0	205.0
50.0	152.0
100.0	114.0
200.0	94.0
300.0	84.0
500.0	74.0
1000.0	58.0

penetration early on. Near 300 years an asymptotic value of approximately 12.0 mm is achieved. The uncertainty bounds (upper) behave similarly, diverging little after this time interval.

4.3 DESIGN OF EXPERIMENTS FOR OPTIMAL UNCERTAINTY REDUCTION

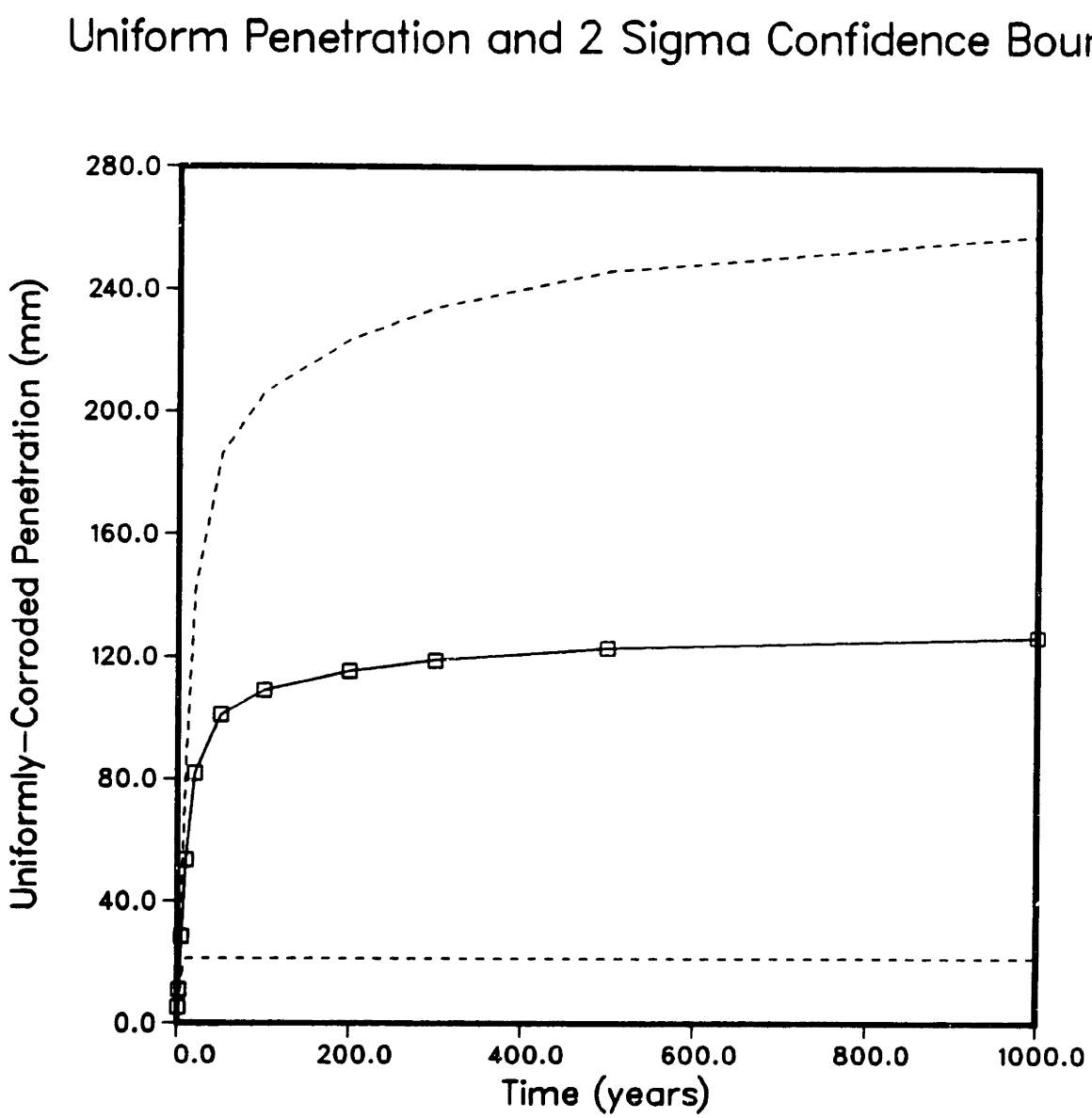
The following section discusses the main results of the thesis, basing the presentation on the application to nuclear waste container penetration by general corrosion. The multivariable model developed above will be used solely to explore the topic of uncertainty-optimized experiment design.

4.3.1 Assignment of Uncertainty to the Virtual Data

The methodology developed in Chapter 3 entails evaluation of a finite sample of potential experiments by generating values for the 'virtual' independent variable associated with a given prescribed potential experiment from the ESS. Thus, a key assumption associated with the methodology is that virtual data (values of the corrosion rate) may be estimated from the model itself. Using the values generated by the model itself, with no error, would drive the uncertainty to zero by including enough virtual data in the MBD. It is absolutely imperative, for the virtual data concept to possess quantitative credibility, to include a consistent measure of error with each of the virtual data in the ESS.

With this in mind, the next two sections discuss the development of a self-consistent model of virtual data error.

Figure 4-13: General Corrosion Penetration and Uncertainty for Commercial High Level Waste Temperature Profile Reference in-service boundary conditions: Temperature profile as given in Table 4-7, O:0.05 ppm, Mg:0.05 w/o, W:0.05 w/f



4.3.1.1 Discussion of the Components of Uncertainty in Predictive Modeling

Vesely and Rasmuson [60] differentiate between two types of uncertainty associated with probabilistic modeling, which are true for predictive modeling in general. They are:

- Uncertainty due to physical variability
- Uncertainty due to lack of knowledge

The first type of uncertainty, as pointed out in their work, is due to actual random behavior in a particular quantity of interest. It is this uncertainty which causes repeated measurements of a specific quantity to yield different values.

The second type of uncertainty, that due to lack of knowledge, results from incompleteness or imprecision in the model itself. Rish [49] identifies this same source of uncertainty, the uncertainty in the formulation of the model itself, as structural uncertainty. The salient feature which distinguishes the two types of uncertainty in predictive modeling is the impact of knowledge on the magnitudes. It is possible to greatly reduce the structural uncertainty with additional knowledge about the physical process, for example, the inclusion of an additional, competing reaction path in a corrosion process model.

Structural uncertainty is far more difficult to assess quantitatively

than physical variability. As has been mentioned previously, the working hypothesis necessary to develop the methods and techniques of this thesis was to assume *The model of general corrosion developed in this thesis is structurally correct, and that it includes all the significant independent variables affecting the corrosion process*, hence this eliminates the 'lack of knowledge' component of the total uncertainty. Based upon the current body of knowledge and data, this model has accounted for observed behavior.

4.3.1.2 An Empirically-Consistent Model of Virtual Data Error

An ideal model of virtual data error would be based, in principle, upon a large sample of data generated at enough combinations of the independent variables so as to characterize the error throughout the variable space represented in the ESS to be evaluated. This is an idealization, however, as it will most often be the case that the ESS will be populated by many experiments which are combinations of the independent variables for which no measured values are available, and which have no quantitative measure of error associated with them. This is the case, for example, when accelerated life testing is being investigated by the UNODEX methodology.

Measurement precision (*e.g.* minimum measurable weight change for a corrosion specimen) may serve as a check on the lower bound of the error, but offers little information to facilitate making an estimate of the physical variability.

One approach taken was to characterize subsets of the MBD for which essentially replicate data existed (with the exception of slight differences in test duration) by fitting the data to various probability distribution functions. Six subsets of the MBD with the greatest sample sizes (from 6 to 15 replicate measurements) were consistently fit to 108 distributions with a software package developed by Christensen [10].

This software tool fits the data to each of 108 data distributions (Christensen [9]), generates descriptive statistics and computes measures of error in central tendency, minima and maxima, width, dispersion, asymmetry and peakedness. These measures of error, which are specific to each distribution, are then weighted and summed into a total measure of error for the fit. Individual weighting factors are adjusted for each candidate distribution so that, as an example, random data generated by a normal distribution produces the least total error for the fitted normal distribution.

Results of this approach indicated, for the data subsets considered, a consistently higher overall ranking given to the more truncated, rectangular distributions (*e.g.* Rectangular, Subbotin, Horseshoe, etc.). The normal distribution consistently appeared in the lower half of the 108 distributions ranked. The exercise provided confirmation that the sparseness of data resulted in too few observations to generate a reliable estimate of the mean and possessed a greater-than-anticipated standard deviation.

The approach taken to remedy the small sample size problem was to formulate a model of the absolute deviation (absolute value of the observed value - calculated value) by linear regression with the MBD. In this way, an empirically-consistent model of error may be generated - based upon actual data - which is functionally dependent upon the independent variable set (for the test conditions).

This same model of error was used to generate estimates of the error in measured values of the MBD, and these errors were, in turn, used as weighting factors for the fit. In this way, an iterative sequence determining the maximum likelihood estimates of the corrosion model and, in turn, the coefficients of the linear regression model of error was performed. The model of error, corrosion rate model and set of parameters and coefficients resulting from the above iteration to convergence (to 1% changes or less) is presented in Table 4-8.

As noted in Section 4.1.1. the average uniform penetration rate is being used as an approximation to the instantaneous corrosion rate. The form of the error model explicitly included the time-dependent contribution so as to follow the kinetic behavior, that is, to vary as the inverse square root of time. This is because it is expected that the error in the mass of metal loss by dissolution will not diverge so rapidly as to become an increasing function of time. Since the error in the penetration is less than linearly increasing with time, but the

instantaneous corrosion rate is approximated by dividing by time, the error in the corrosion rate is expected to decrease in time.

4.3.2 Specification of the Experiment Sample Space

The technique of discretizing the population of all conceivable potential experiments into what has been termed the Experiment Sample Space will be reviewed below.

The UNODEX methodology of evaluating potential experiments for their value in reducing the uncertainty in the prediction of waste container penetration by general corrosion makes the following assumptions:

- The operable mechanism of general corrosion in the repository environment is preserved for all the test conditions established in the ESS. This is often stated as a constraint upon any type of accelerated life test.

- The model of general corrosion formulated above in Table 4-4 is structurally correct, and adequately describes the physical process for the entire independent variable space defined by the ESS, the MBD and the expected in-service conditions.

The following paragraphs present the logic for specification of the ESS virtual data ranges are specified.

Regarding the temperature range, the maximum limit was specified at the temperature of 220°C was selected, based upon early thermal calculations for CHLW, referenced in Section 2.3.1. This maximum container-salt interface temperature has been calculated more recently and is documented in Table 4-7 above, indicating the maximum value of

Table 4-8: Convergence Steps in Obtaining the Empirically-Consistent Model of Virtual Data Error

Iteration=	1	2	3	4	5	6
a_1	1.26714	1.27492	1.27381	1.27400	1.27398	1.27402
a_2	-21.3949	-15.8527	-15.3725	-14.9748	-14.8374	-14.7625
a_3	692.679	671.829	623.132	606.015	598.121	595.031
a_4	-0.21545	-0.15086	-0.14904	-0.14557	-0.14454	-0.14388
b_1	1.289+11	7.978+10	7.986+10	8.042+10	8.045+10	8.067+10
b_2	774.458	464.925	463.774	466.528	466.406	467.604
b_3	16243.59	16178.22	16139.07	16122.15	16115.05	16111.85

$$E = a_1 T + a_2[O] + a_3[Mg] + a_4[H_2O] + \frac{a_5}{\sqrt{t}}$$

$$y = \frac{b_1}{b_2 + \sqrt{t}} \times exp\, c_1[O] + c_2[H_2O] + b_3[Mg] - \frac{c_4}{T}$$

227°C at 5 years. There is no published literature regarding any dominant mechanism different than that exhibited in the MBD measurements at these temperatures (150°C - 220°C).

The minimum temperature was selected to reflect ambient temperatures at the repository horizon, approximately 60°C.

Dissolved oxygen concentrations are expected to become anoxic (0.05 ppm) shortly after permanent closure. However it is conceivable that a waste container may be subject to contact with aerated brine for the entire operating period, as the degree to which brine will be aerated depends upon the rate of creep closure of the salt upon the container and the sealing capability of the salt against oxygen diffusion.

The maximum dissolved oxygen concentration was assumed to be 2.0 ppm for the ESS, in the interest of obtaining overstress test information on this variable.

Magnesium concentration limits were set at 0.001 and 0.06, reflecting concentration values of PBB3 (0.059) for the maximum value, and representing the dissolution scenario, in which 98.4 weight percent of the total brine derives from dissolution of the bedded halite and the remaining 1.6 weight percent from the included high-magnesium brine for the minimum value (0.984*0.0001 + 0.016*0.059 = 0.001).

Total water fraction is specified at the limiting values of 5.0 weight percent (lowest test value) and 80.0 weight percent, corresponding to all brine (20.0 percent are dissolved solids) at the wetted surface.

Table 4-9 summarizes the above specifications for the ESS.

With the model of general corrosion, the experiment sample space and the in-service environment specified, it is now possible to generate uncertainty-optimized experiment designs.

4.3.3 Notation and Review of UNODEX

In all the experiment designs which follow, a shorthand notation will be adopted which uniquely identifies each potential experiment in the ESS under evaluation. Each experiment in the ESS has associated with it a unique 5-digit number composed of a 'level number' in each position 1 through 5 (left to right). The positions directly correspond to (1) Temperature, (2) Dissolved Oxygen Concentration (3) Magnesium Concentration, (4) Total Water Fraction and (5) Time, or duration of the test. The level numbers are assigned, starting from one (corresponding to the lowest value of the independent variable) and ranging to the number of discrete levels which that particular independent variable may assume. Hence for an ESS with limits on the independent variables as indicated in Table 4-9, and three (3) equispaced levels per independent variable, the virtual data number 11132 would correspond to a potential experiment conducted at the lowest level for temperature, 60°C, the

Table 4-9: Limiting Values for the Experiment Sample Space

Independent Variable	Minimum	Maximum
Temperature (°C)	60	220
Dissolved Oxygen (ppm)	0.05	2.0
Magnesium Concentration (w/f)	0.0001	0.06
Total Water Fraction (w/f)	0.05	0.80
Test Duration (hours)	750	20,000

lowest level for dissolved oxygen concentration of 0.05 ppm, the lowest level for magnesium concentration, that being 0.001 w/f, and to the highest level for water fraction 80 w/o, and the mid-level for time; (20,000 + 750)/2 = 10,375 hours.

In the interest of exploring general effects and reducing complexity of data presentation, for the most part the ESS's investigated will be limited to 2 levels per variable. Hence only the extrema will be considered. This results in 2^5 = 32 virtual data representing potential experiments.

By way of quick review, the UNODEX methodology will be highlighted in this paragraph. Recall that the elements of the methodology are: a model building database (MBD), a virtual data experiment sample space (ESS), a multivariable model of general corrosion, a model of error due to physical variability as dependent upon the same independent variable set used in the corrosion model, and an estimate of the time-dependent behavior of the independent variables for the in-service environment. UNODEX assembles the above elements so that the following sequence of computations may be performed:

1. The corrosion model is fitted with maximum likelihood estimates of the unknown model parameters and errors, based solely upon the MBD.

2. The uncertainty at the desired design life (300 or 1000 years) is calculated and referenced as the benchmark penetration and uncertainty.

3. Virtual data from the ESS are sequentially evaluated, by shifting one virtual data point into the MBD, calculating the improvement in uncertainty based upon new parameter estimates (and errors), and shifting the virtual data point back out of the MBD again. This continues until each virtual data point in the ESS has an uncertainty reduction associated with it.

4. The virtual data are then cumulatively added to the MBD, in rank order, and the total reduction based on the cumulative addition is calculated at each step (*i.e.* the uncertainty reduction based on the addition of the first of the virtual data points, the first and second, the first, second and third, etc.).

5. After the ESS is evaluated cumulatively, based on the first ranking, the profile of the above uncertainty vs. number of experiments added is evaluated for the presence of a plateau, followed by a sharp discontinuity (section 4.3.5 discusses this phenomena in greater detail) and when this is found, all virtual data up to the point of the plateau are shifted into the MBD, the remaining virtual data are reevaluated sequentially as in 3. above.

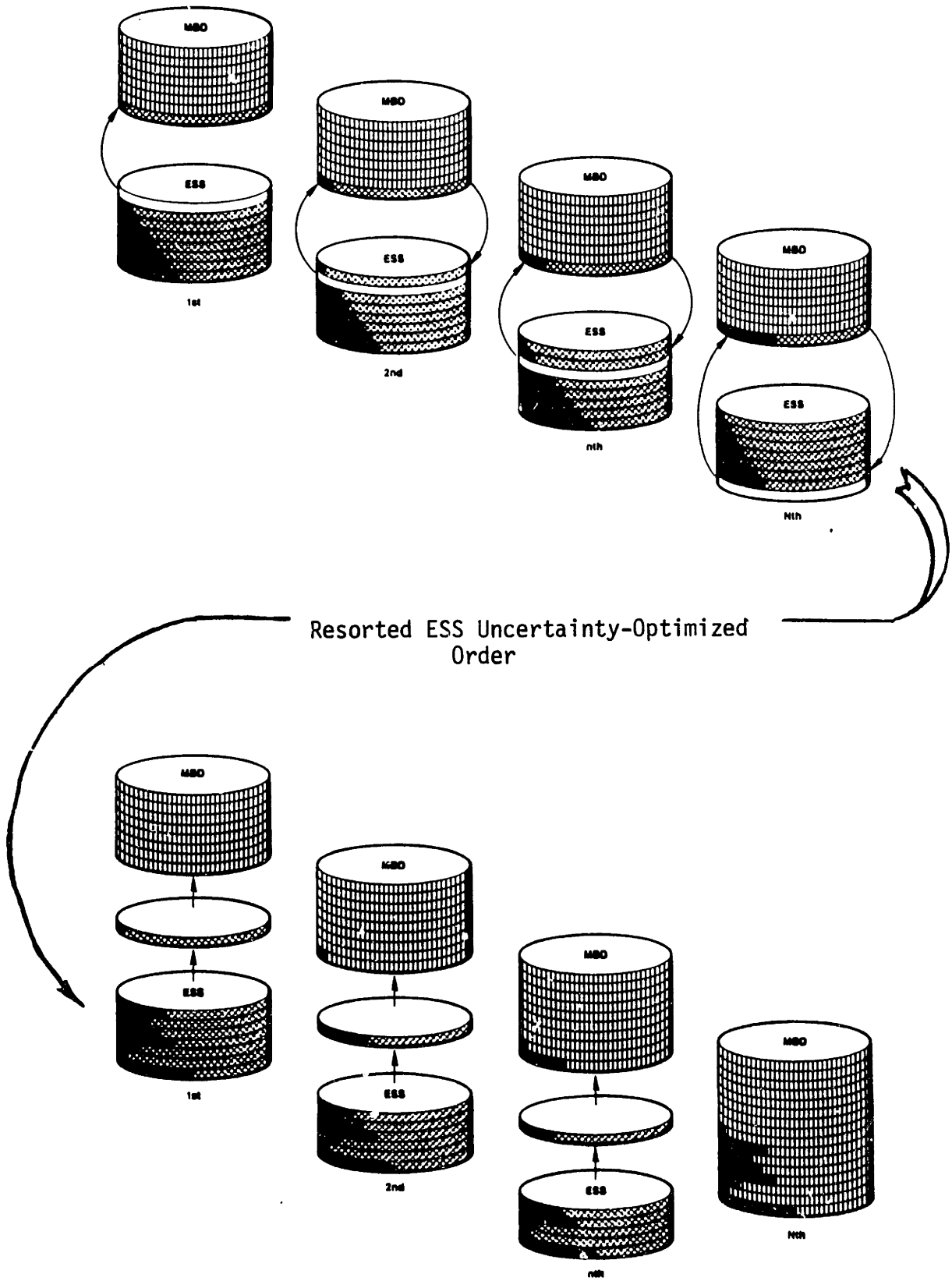
6. This generates the total uncertainty reduction vs. number of experiments added, in Uncertainty-Optimized (UO) order.

The same information is displayed in Figure 3-3. Figure 4-14 illustrates the sequential swapping and cumulative addition of the virtual data into and from the MBD.

4.3.4 Validation of the Methodology

As a first exercise to apply the UNODEX methodology, and to gain the most readily achievable confidence (validation) in the predicted results, the straightforward application is made to evaluating an ESS which is limited to the same independent variable space as the MBD

Figure 4-14: Illustration of the Data Handling Steps in the UNODEX Methodology



itself. This application allows a pseudo-benchmarking of the results by determining the improvement in uncertainty due to the addition of more of the same type of data which was used to parameterize the model itself. It is intuitive that there should be no great improvement in the uncertainty at 300 years (chosen as the arbitrary design life for investigation) even with the total addition of essentially replicate data to the MBD. The reasons for improvement by this addition are due to the increased number of data and the less severe error in the virtual data as compared to the few outliers in the model building data which contribute significantly to the error.

The results of this evaluation do indeed confirm the expected results, as Figure 4-15 indicates. This figure displays the uncertainty at 300 years as a function of the added experiment number. Experiments are added in the uncertainty-optimized order, as defined above. The reference ESS values for the low levels (Table 4-9) were used, but the high levels for all the variables were held to the mean values for the MBD. These are: temperature 144°C, DO 0.0154 ppm, Mg 0.014 w/f, water fraction 41.8 w/o and test duration 2376 hours.

Total reduction in uncertainty for the addition of the 32 virtual experiments amounts to less than 1 mm. The uncertainty-optimized order of the experiments is presented as Table 4-10.

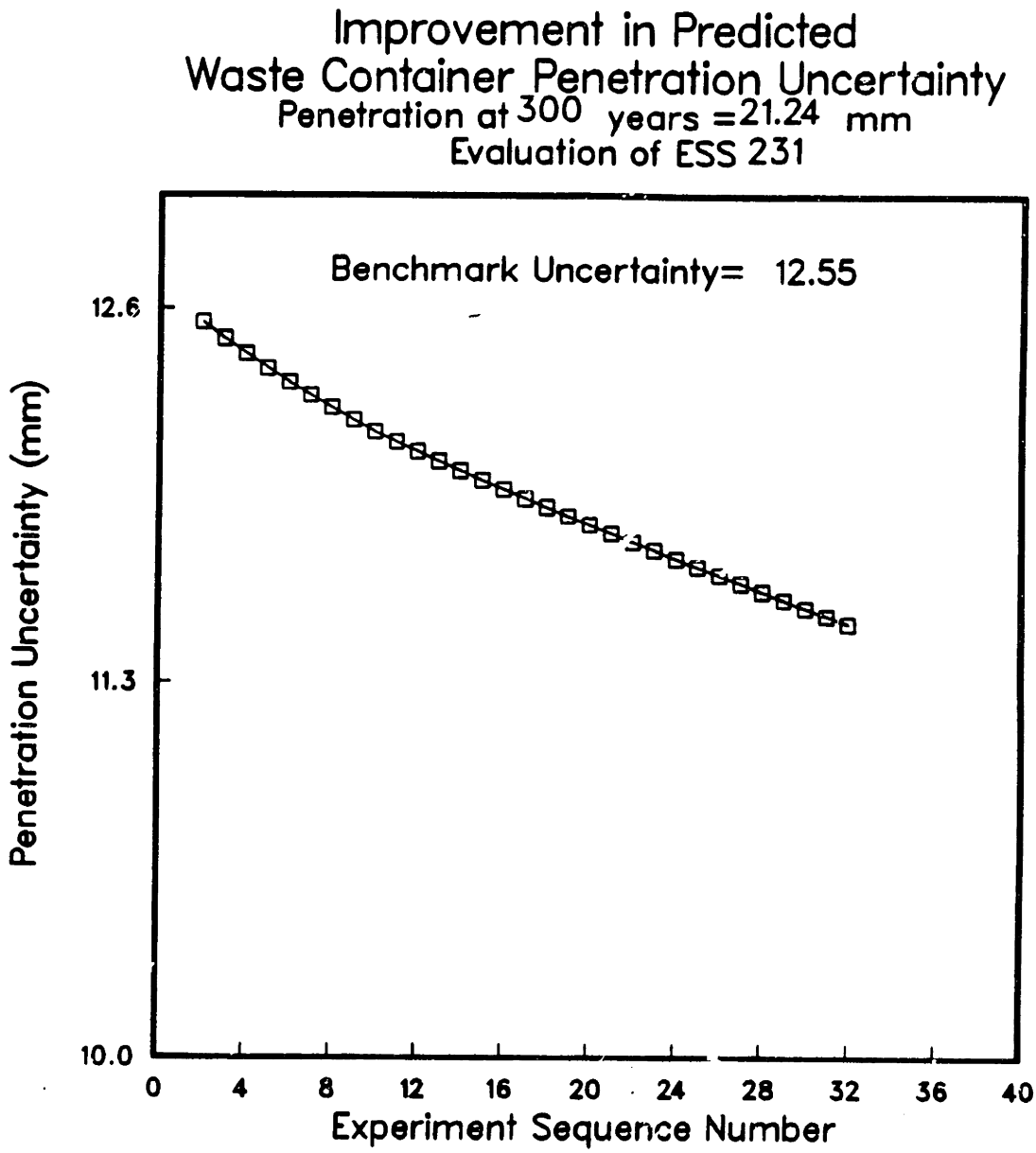
Table 4-10: Uncertainty-Optimized Design for the Validation Exercise

No.	$\Delta\sigma_D$ (μm)	σ'_D (μm)
22221	5.649609E+01	1.249616E+04
21221	8.605237E-03	1.244463E+04
22211	1.583965E+02	1.239426E+04
21211	2.080244E+02	1.234463E+04
22121	2.528760E+02	1.229978E+04
21121	2.966465E+02	1.225601E+04
22111	3.403223E+02	1.221233E+04
21111	3.825566E+02	1.217010E+04
22222	4.168857E+02	1.213577E+04
21212	4.498223E+02	1.210283E+04
21222	4.833291E+02	1.206932E+04
22212	5.156807E+02	1.203697E+04
12221	5.475293E+02	1.200512E+04
11221	5.795283E+02	1.197313E+04
11121	6.104717E+02	1.194218E+04
11111	6.411768E+02	1.191148E+04
22112	6.715615E+02	1.188109E+04
11122	7.017432E+02	1.185091E+04
12212	7.321064E+02	1.182055E+04
12222	7.617949E+02	1.179086E+04
12211	7.913740E+02	1.176128E+04
21112	8.207051E+02	1.173195E+04
12121	8.494199E+02	1.170323E+04
12111	8.783096E+02	1.167434E+04
11211	9.065811E+02	1.164607E+04
11212	9.350127E+02	1.161764E+04
12112	9.632686E+02	1.158938E+04
11112	9.908730E+02	1.156178E+04
12122	1.018683E+03	1.153397E+04
11222	1.045891E+03	1.150676E+04
21122	1.073510E+03	1.147914E+04

$\Delta\sigma_D$ = *Uncertainty Reduction (D = 300years)*

σ'_D = *New Error (D = 300years)*

Figure 4-15: Uncertainty Reduction for the Validation Exercise ESS



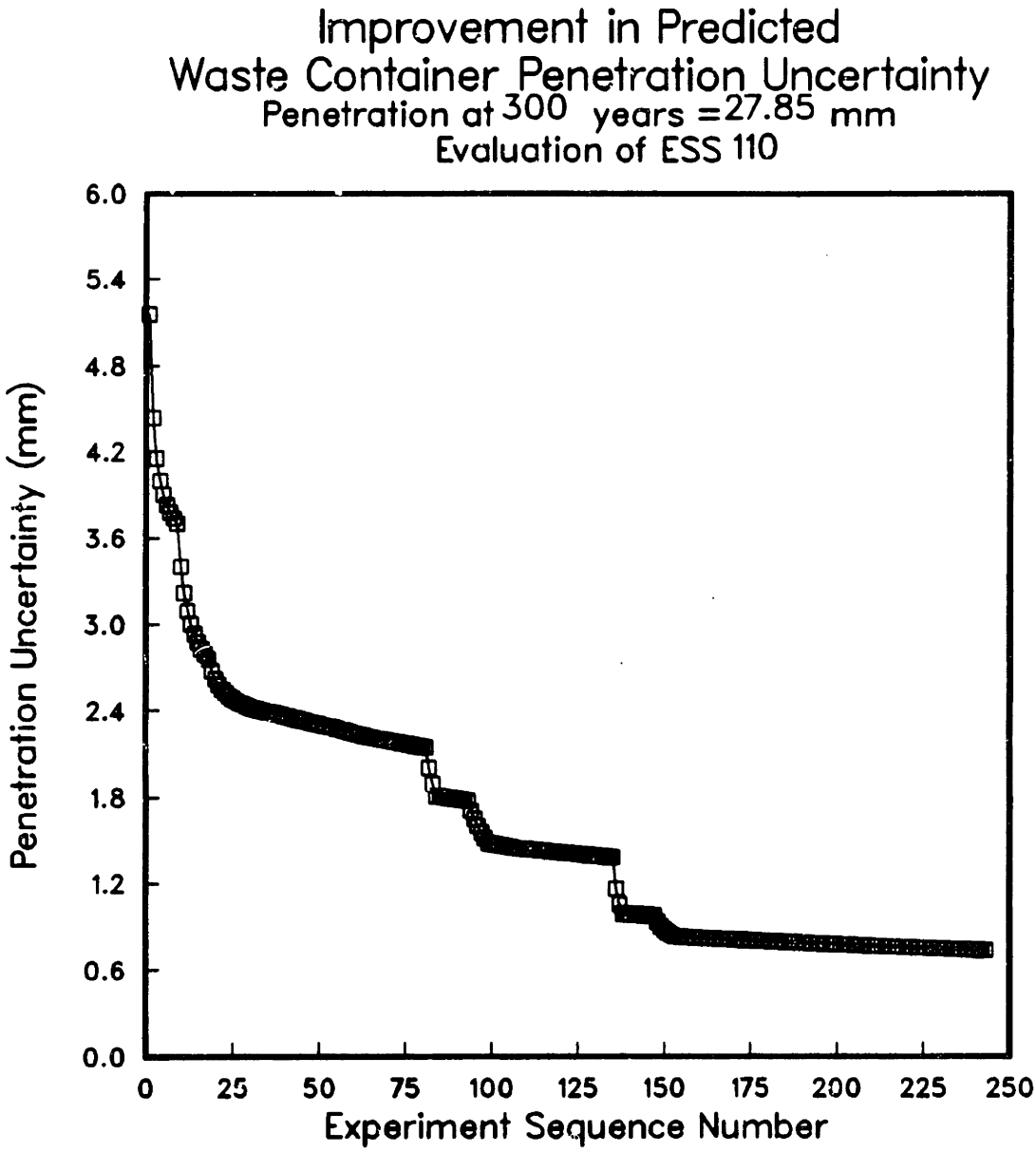
4.3.5 The Resequencing Frequency

One of the most interesting aspects of the UNODEX methodology has already been alluded to in the above descriptions of the computation sequence. Addition of all the virtual ESS data in the initially-sorted uncertainty-optimized order results in a pronounced discontinuous behavior in the plot of uncertainty vs. sequence number. One computation of such behavior is presented as Figure 4-16. The ESS specified for this application was the same as we have been calling the reference case (Table 4-9), except the number of levels per independent variable was chosen as 3 in order to better illustrate the behavior in 243 points.

Figure 4-16 serves only to illustrate the discontinuities which may occur if resequencing is not employed. It does not represent quantitatively correct penetration and uncertainty, as no error weighting scheme was used to generate the results in this figure. For comparative purposes, Figure 4-17 presents results generated by resequencing the virtual ESS data after the 1^{st}, 2^{nd}, 10^{th} and 125^{th} experiment, based upon an algorithm in UNODEX which resequences the remaining virtual data upon detection of a plateau ('knee' in the curve).

This test algorithm steps through the incremental uncertainty difference vs. experiment number data, comparing the slope at a given

Figure 4-16: Uncertainty Reduction for the Case of no Resequencing



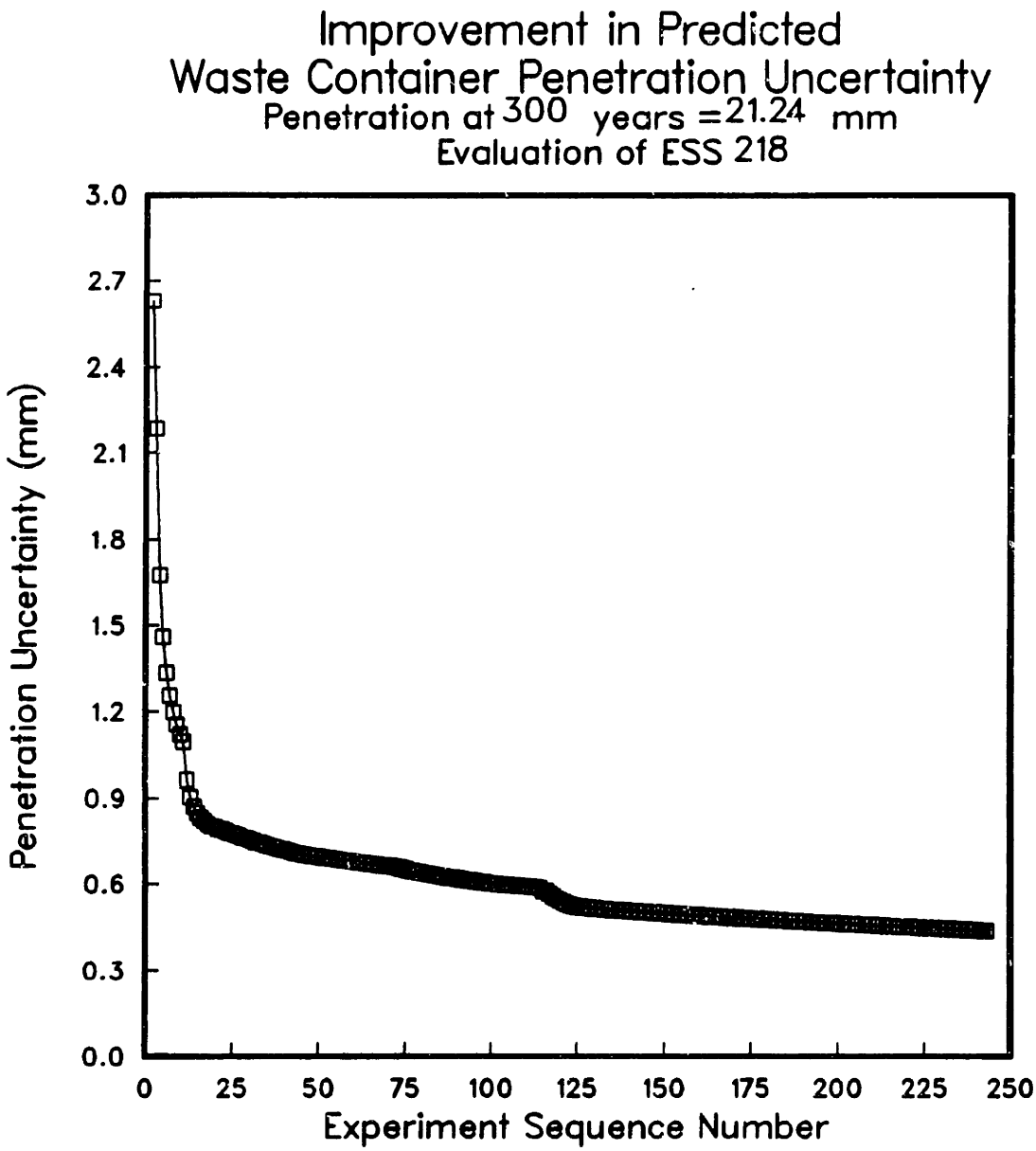
point to the average of the three previous slopes. When the quotient of the new slope and the three-point-average falls below a predetermined criterion, (input parameter, in this case 0.20) the virtual data in ranked positions greater than the test value are all resequenced, by sequential evaluation.

4.3.6 Accelerated Life Testing and the First Point Uncertainty Reduction

One of the primary conclusions of this thesis will be discussed in this section, that of the 'first point uncertainty reduction'. This section addresses itself to quantitatively evaluating accelerated life testing. The linkages established between model, data, virtual data and error provide the means to address accelerated life testing in a single variable at overstress conditions and for multiple variables at overstress test conditions.

Results of the reference ESS (for 2 levels per variable) are presented as Figure 4-18. The most striking feature of this evaluation is the magnitude of the uncertainty reduction associated solely with the addition of the first virtual data point. The penetration and uncertainty at 300 years based only on the MBD, the 'Benchmark Uncertainty', are 22.29 mm and 13.84 mm, (standard deviation) respectively. Table 4-11 accompanies the figure. It can be noted from the table that the first virtual data point, ranked the greatest for uncertainty reduction, is at all high levels of the independent

Figure 4-17: Uncertainty Reduction with Resequencing at Points 1, 2, 10, 125



variables, namely point 22222. Uncertainty is reduced from 13.84 mm to 2.98 mm, or 78%. This counterintuitive result deserves some further explanation. The reference ESS conditions specify this point at a test duration of 20,000 hours, roughly an order of magnitude times the mean MBD test duration of 2376 hours. As well, all other variables, when at the maximum value represent a temperature, DO level and magnesium concentration which is unrepresented in the MBD.

It should be noted that the model contains data with test durations ranging from 300 to 7,000 hours, with a mean test duration of 2376 hours, hence the simulated test at 20,000 hours is a very long term test which becomes more important to extrapolations than the bulk of the MBD which is clustered at relatively short times.

Also, the test is an accelerated life test in all variables relative to in-service conditions, and with the functional relationship among the independent variables available via the corrosion rate model, the overstress conditions in the non-time independent variables in effect act to simulate a longer term test.

This large reduction in uncertainty may be explained in terms of the uniqueness of the test and hence the associated information gain due to this uniqueness. The first data point introduced is at an entirely new coordinate in the independent variable space. The information gain in

Figure 4-18: Results of Uncertainty Reduction for the Reference ESS

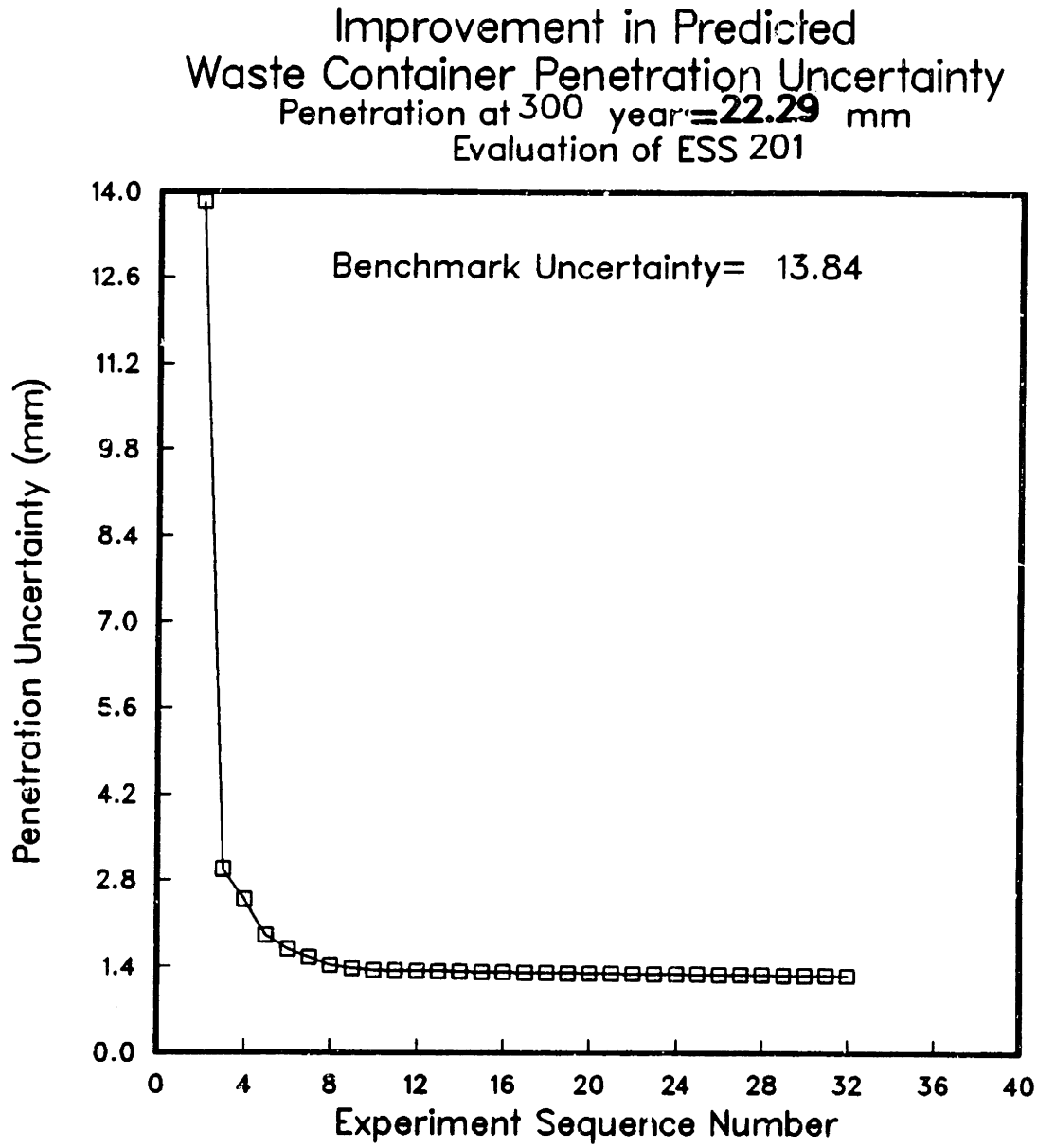


Table 4-11: Tabulation of Uncertainty Reduction for the Reference ESS

No.	$\Delta\sigma_D$ (μm)	σ'_D (μm)
NONE		1.383987E+04
22222	1.086304E+01	2.976828E+03
22221	4.913547E+02	2.485474E+03
22212	5.699739E+02	1.915500E+03
21222	7.998251E+02	1.685649E+03
21212	9.323374E+02	1.553136E+03
22211	1.057440E+03	1.428034E+03
21221	1.110567E+03	1.374907E+03
21211	1.141975E+03	1.343499E+03
22122	6.111450E+00	1.337388E+03
22112	1.151111E+01	1.331988E+03
21122	1.662024E+01	1.326879E+03
21112	2.121997E+01	1.322279E+03
22121	2.778760E+01	1.315711E+03
22111	3.349988E+01	1.309999E+03
21121	3.864783E+01	1.304851E+03
21111	4.343325E+01	1.300066E+03
12222	4.696619E+01	1.296533E+03
12212	5.042419E+01	1.293075E+03
11222	5.372473E+01	1.289774E+03
11212	5.705945E+01	1.286440E+03
11121	6.028552E+01	1.283214E+03
12111	6.347546E+01	1.280024E+03
12121	6.665405E+01	1.276845E+03
11122	6.979736E+01	1.273702E+03
11111	7.292334E+01	1.270576E+03
12112	7.603174E+01	1.267467E+03
12221	7.912524E+01	1.264374E+03
12112	8.225342E+01	1.261246E+03
12211	8.529626E+01	1.258203E+03
11211	8.823401E+01	1.255265E+03
11221	9.132251E+01	1.252177E+03

$\Delta\sigma_D$ = *Uncertainty Reduction (D = 300years)*

σ'_D = *New Error (D = 300years)*

the addition of a replicate data point doubles the local information, raising it from 1 to 2, while the gain in information in adding a unique data point raises the local information from 0 to 1. The absolute increase is the same, but the relative increase is essentially infinite. Based upon this interpretation, subsequent additions of data with similar independent variable values yield far less uncertainty reduction.

An exercise may be performed which generates the reduction in uncertainty due to this unique, first point as a function of the maximum test duration. Figure 4-19 presents the fractional reduction of the benchmark uncertainty due to this 'first point addition' presented functionally against maximum test time. The upper line on the curve is for 1000 year design life and the lower line is for 300 years. The results exhibited by this curve are far reaching. If a commitment is to be made to use accelerated life testing, the results presented here serve to quantify the benefit of longer test times, and provide numerical input to optimization analyses, such as the cost of uncertainty reduction.

The same type of results are tabulated for temperature in Figure 4-20. Results indicate that, for a fixed maximum test duration of 20,000 hours, the fractional uncertainty reduction due to 'first point' addition is nearly linear with maximum temperature.

Figure 4-19: First Point Uncertainty Reduction vs. Test Duration

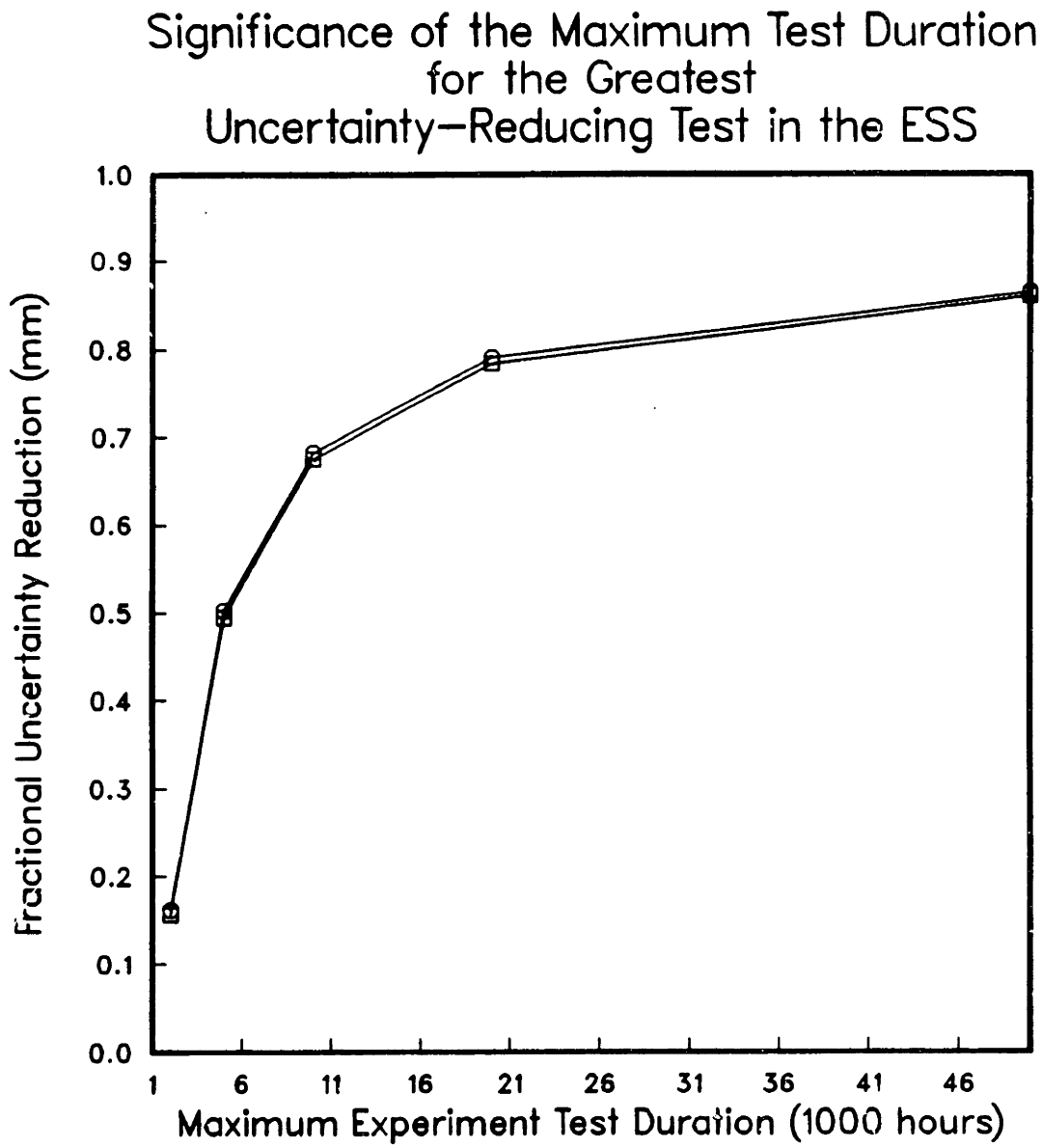
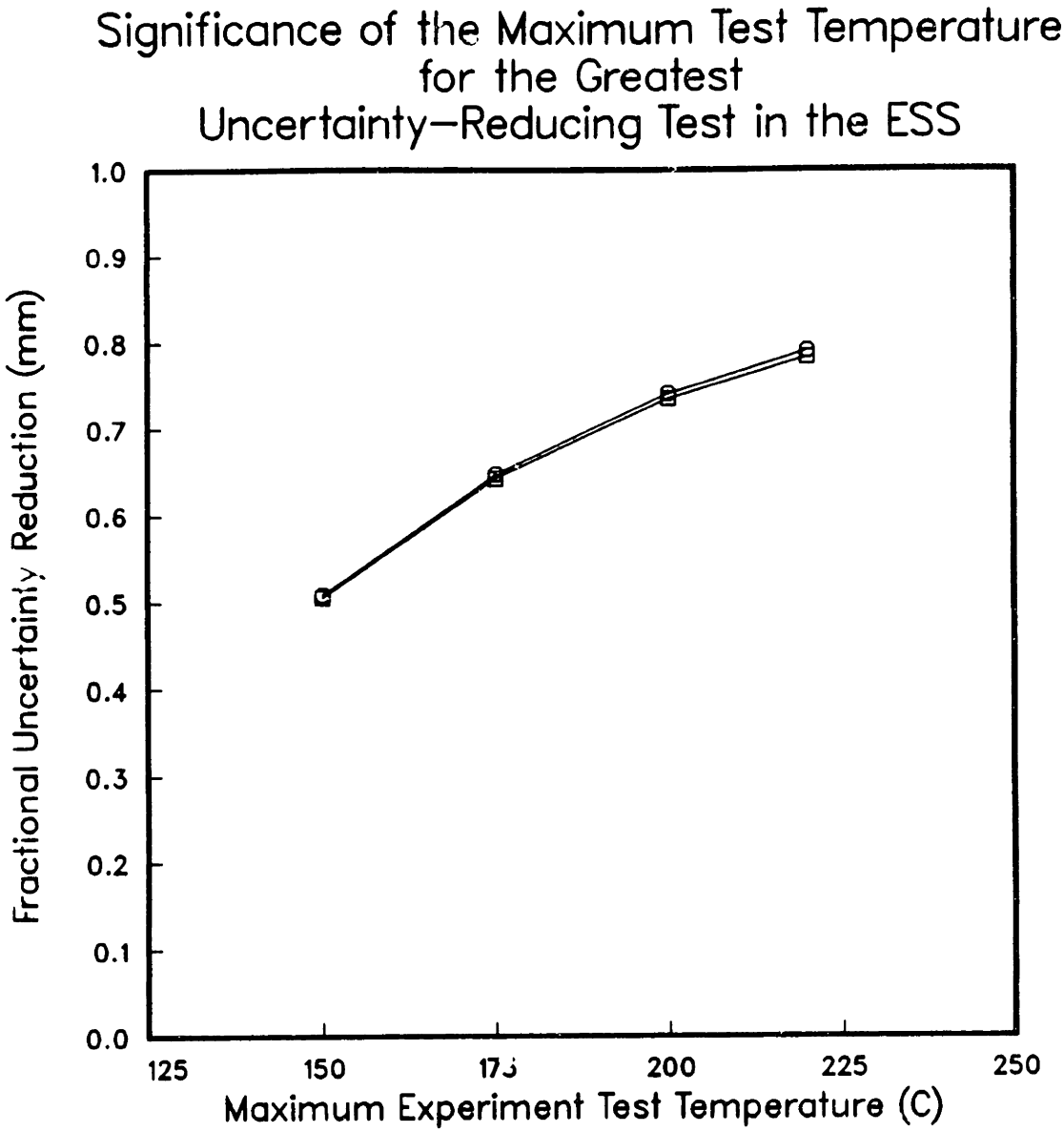


Figure 4-20: Uncertainty Reduction Dependence on Test Temperature for Multivariable-Accelerated Experiments

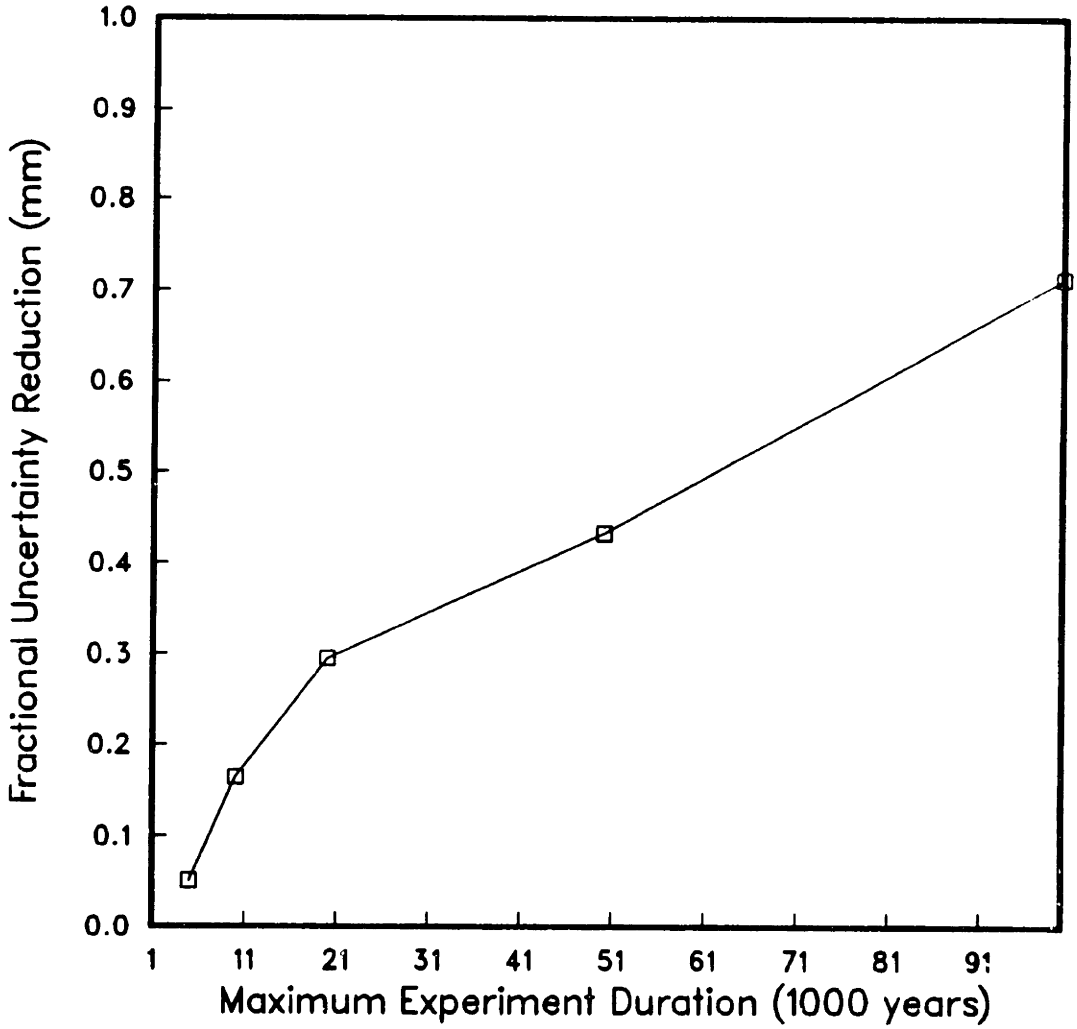


If there is some error in the structural form of the multivariable corrosion model, then the variable interactions may not be quantified correctly, and accelerated life testing in more than one overstress variable would not be appropriate. However, since the model describes the MBD adequately, it is possible to analyze the same type of behavior as above, while holding the maximum value for all but the overstress variable at the MBD mean values. This univariate accelerated life testing first point uncertainty reduction is displayed in Figure 4-21. As can be seen by comparing Figure 4-21 with Figure 4-19, single variable (thermal) accelerated life testing will require 100,000 hours of testing to generate approximately the same 'first point' uncertainty reduction as will accelerated life testing in all the independent variables for 10,000 hours. This order of magnitude difference in test duration clearly indicates the impact of successful accelerated life test data on total data requirements and the imperative need for a valid, detailed corrosion process model.

4.3.7 Overall Trend in Uncertainty-Optimized Designs

Finally, as a complimentary analysis to the above 'first point' uncertainty results the uncertainty-optimized experiment designs will be analyzed for general trends in the reference ESS and exercises are performed to determine the limits of these general trends in the following section.

Figure 4-21: Uncertainty Reduction Dependence on Test Duration for Thermally-Accelerated Experiments



4.3.7.1 Reference ESS

The uncertainty-optimized design for the reference ESS is presented as Table 4-12, following. Virtual data ESS numbers appear in the final, optimized order, after resequencing at the 1st, 2nd and 8th virtual data point addition. The second column of the table presents the uncertainty at 300 years based upon the addition of all the virtual ESS data, cumulatively, up to the ESS number in the first column. The final columns list the calculated value for the corrosion rate, and the associated virtual data error.

As can be seen in the table the uncertainty-optimized design is constructed so that all of the high temperature data points rank greater than that obtained at lower temperatures which strongly indicates the overall importance of the test temperature in controlling uncertainty. The corrosion rate falls off monotonically and the error increases monotonically with decreasing uncertainty reduction for contiguous groups of data sharing a common test duration. In general then, for a fixed test time, low error, high corrosion rate experiments consistently rank the most favorable and low corrosion rate, high error experiments the least favorable.

Consistency in the trend is greatly diminished after the transition into the low temperature tests. The low temperature tests populate the very flat portion on the uncertainty-experiment curve. Differences in

Table 4-12: The Uncertainty-Optimized Experiment Design for the Reference ESS

No.	$\Delta\sigma_D$ (μm)	σ'_D (μm)	y (μm/yr)	E (μm/yr)
22222	10863.04	2976.828	7420.586	276.1801
22221	491.3547	2485.474	9129.373	281.2977
22212	569.9739	1915.500	7420.525	286.9709
21222	799.8251	1685.649	7420.519	304.9669
21212	932.3374	1553.136	7419.980	315.7578
22211	1057.440	1428.034	9129.582	292.0886
21221	1110.567	1374.907	9129.812	310.0846
21211	1141.975	1343.499	9129.573	320.8755
22122	6.111450	1337.388	1079.122	241.0732
22112	11.51111	1331.988	1079.122	251.8641
21122	16.62024	1326.879	1079.121	269.8601
21112	21.21997	1322.279	1079.121	280.6509
22121	27.78760	1315.711	1327.774	246.1909
22111	33.49988	1309.999	1327.774	256.9818
21121	38.64783	1304.851	1327.772	274.9778
21111	43.43323	1300.066	1327.772	285.7686
12222	46.96619	1296.533	67.24272	72.33686
12212	50.42419	1293.075	67.23022	83.12771
11222	53.72473	1289.774	67.23260	101.1237
11212	57.05945	1286.440	67.23255	111.9146
11121	60.28552	1283.214	4.763974	71.13458
12111	63.47546	1280.024	4.763733	53.13856
12121	66.65405	1276.845	4.763735	42.34771
11122	69.97936	1273.702	3.871200	66.01690
11111	72.92334	1270.576	4.763800	81.92543
11112	76.03174	1267.467	3.871825	76.80775
12221	79.12524	1264.374	82.72289	77.45454
12112	82.25342	1261.246	3.871831	48.02088
12211	85.29626	1258.203	82.72179	88.24539
11211	88.23401	1255.265	82.71934	117.0323
11221	91.32251	1252.177	82.74504	106.2414

$\Delta\sigma_D$ = *Uncertainty Reduction (D = 300years)*

σ'_D = *New Error (D = 300years)*

virtual data in this region of the ESS are very small, and the various experiments essentially contribute an equivalent uncertainty reduction.

The most interesting feature of the the uncertainty-optimized design is that the general trend is found to exhibit an oscillatory behavior in ranking long- and short-term data. As can be seen in the table, (see also the discussion in Section 4.3.6. above) the optimal experiment to perform first is the most unique experiment, the one which is the furthest from MBD in independent variable space. This point will be at the highest of the overstress conditions, and will yield the greatest corrosion rate and penetration. Due to the structure of the empirical error model (Table 4-8), this virtual data point also has a relatively small predicted error.

The addition of subsequent virtual data would appear to involve a simple rank ordering of those remaining points which would, each in turn, yield the greatest corrosion rate with the least error. This, however, is not the case. The complication arises when one considers that the addition of the first virtual data point to the MBD (it now becomes the same as a measured experimental observation) determines a new IV space. The next greatest uncertainty-reducing experiment will be the most unique, measured against the MBD plus the newly added virtual data.

Because the required extrapolation is in time* to the desired design life, the optimal order of addition of virtual data will be driven by obtaining the greatest confidence in the time dependence of the corrosion rate. This is what leads to the oscillatory trend in ranking long- and short- term data.

Table 4-13 displays the first 16 (high temperature) virtual data from the uncertainty-optimized design of Table 4-12 above. This tabulation uses the independent variable names instead of the shorthand notation and is structured to expose the repeating trend. From this table (or Table 4-12) it can be seen that the calculated corrosion rate decreases from its value at all high IV levels, by reducing to the low level, the following independent variables:

$$W > O > (W+O) > Mg > (W+Mg) > (O+Mg) > (W+O+Mg)$$

in the indicated order.

The table indicates the first virtual data point is at all high levels. The first oscillation occurs when the second data point is added and all variables are held high, except time. The subsequent optimal additions are long time tests which reduce the corrosion rate by the smallest amount in each step, reducing water, dissolved oxygen, and

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*Note that *time* is the only variable which exceeds the range established by the ESS in the in-service environment.

both water and dissolved oxygen in sequence. The same sequence of three is repeated at short times, and then the magnesium level is reduced and the W, O, W+O sequence is repeated for long and short times.

This trend behavior is exhibited for ESS's about the reference case for a maximum test time of approximately 50,000 hours and a minimum of from 5,000 to 10,000 hours. The longer test times cause the corrosion rate to decrease such that high levels for the other variables act effectively to accelerate the degradation more than the actual test time and hence the uncertainty-optimized order of the reference case is not preserved exactly. As the maximum test time becom ; too short, of the order of the mean for the MBD, long term tests become noncontributing.

4.4 SUMMARY

Summarizing, the main results of the thesis were presented in this chapter, the application of the uncertainty-optimized experiment design to waste container penetration.

In the process of accomplishing this goal, the body of experimental data relevant to the brine-steel corrosion system to be encountered in the repository was evaluated. It was found that only nuclear waste program specific-data would provide satisfactory detailed information. The data from various types of tests were reviewed and consolidated into a single database from which to generate maximum likelihood estimates of corrosion model parameters.

Table 4-13: Oscillatory Nature of the Overall Trend in Uncertainty-Optimized Designs

UO Number	Long Term Tests	Short Term Tests
1	- All Independent Variables at High Levels -	
2		t
3	W	
4	O	
5	W + O	
6		W + t
7		O + t
8		W + O + t
9	Mg	
10	W + Mg	
11	O + Mg	
12	W + O + Mg	
13		Mg + t
14		W + Mg + t
15		O + Mg + t
16		W + O + Mg + t

Various investigations of compatible subsets of the above and other relevant data were performed to determine the principle variables which should compose a multivariable model of general corrosion. Based upon separate effects behavior and fundamental principles of similar chemically-driven degradation processes, several test models were constructed. Based solely upon the performance of the alternative models when fitted to the database, the superior model was selected. The sensitivity of this model to various nonlinear regression controls, such as convergence criteria, weighting factors and starting guesses, was assessed, and the model found to be satisfactory, even when two of the five parameters were fixed as constants.

Assumptions regarding the expected time dependence of the in-service environment were made, and resulting time- and environment-integrated penetration and uncertainty were calculated for the assumed reference case and several known potential perturbations from the reference case.

Finally, the impact of a performing a wide array of potential experiments was assessed for impact on uncertainty reduction at 300 and 1000 year design lives. The concept and techniques of simulating 'virtual' data are developed and the methodology is effectively validated by comparing the uncertainty reduction for the 'virtual' data against the actual measured data in the database. Accelerated testing in one (temperature) and multiple control variables was quantitatively

evaluated. Two primary techniques which evaluate potential experiments are developed and results presented; 'first point' uncertainty reduction and overall trend in uncertainty-optimized designs.

The primary results of this application are:

- Optimization of the experiment design requires multiple passes at resequencing the virtual ESS data.

- The uncertainty-optimized experiment design always exhibits a large reduction in uncertainty associated with the most unique (as compared to the model building database) overstress experiment. In this sense, accelerated life testing is identified as viable.

- Quantitative evaluations of the uncertainty reduction associated with multivariable accelerated life testing indicate a strong nonlinear uncertainty reduction with total test duration.

- Overall trend behavior for uncertainty-optimized designs indicate a strong tendency to oscillate between repeated sequences of long- and short-term tests. This is driven by the necessity of establishing the corrosion rate vs. time behavior at the test time extrema, thus enabling the most confident extrapolation.

The entire application necessarily makes the working hypothesis that: *The model of general corrosion developed in this thesis is structurally correct, and that it includes all the significant independent variables affecting the corrosion process.* In fact, knowledge of the waste container corrosion process is not complete at all, and dealing with that uncertainty will necessitate, in addition to further fundamental research, the implimentation of the UNODEX methodology with many different corrosion rate models.

5. SUMMARY, CONCLUSIONS AND RECOMMENDATIONS FOR FUTURE STUDY

5.1 INTRODUCTION

The history of developments within the nuclear fuel cycle, particularly the more recent policy decisions regarding antiproliferation have effectively locked the light water reactor into a most inefficient operating mode, the 'once-through' fuel cycle. One significant consequence of this type of wasteful nuclear energy economy is the problem of disposal of rapidly accumulating spent fuel.

The passage of the Nuclear Waste Policy Act of 1982 [57], has, with some urgency, charged the US Department of Energy with the responsibility of administering the nation's effort for ultimate disposal of High-Level Nuclear Waste in mined geologic repositories.

Federal regulators have been motivated particularly by the large inventory (70,000 MT) of radioactive material intended for disposal in this potential repository, and the long term radiological threat that such an inventory could potentially pose to the human environment for many generations, to develop regulations applicable over thousands of years. Specific federal regulations have been written, one of which focuses on providing an early containment of radionuclides within engineered waste containers for from a minimum of 300 to 1000 year time periods. The logic behind this time particular time period is that it roughly coresponds with the time interval during which radioactivity and

heat generation are dominated by the decay of fission products (most notably Cs^{137} and Sr^{90}). Most physical and chemical changes to waste package components which can potentially affect mechanical stability and isolation are at their highest during the first 1000 years.

Since no permanent high-level nuclear waste repository has ever been built or operated, and in light of the above mentioned long design lives, assessment of performance will require extrapolation beyond existing technical experience. Regulators have recognized that the unique difficulties associated with credible validation of performance predictions over 1000 year container design lives demand a unique experimental treatment. Specifically, federal regulations call for the use of accelerated tests; "Demonstration of compliance ...will involve the use of data from accelerated tests and predictive models..."*.

5.2 PURPOSE OF THE WORK

The stated purpose of this work has been to quantify the impact that additional experimental data may provide on the uncertainty in nuclear waste container penetration predictions, before these experiments have actually been performed. By developing a methodology to accomplish this task, the techniques to design an experimental test matrix ranking (from a pre-specified collection of potential experiments) the candidate tests under evaluation from greatest to least uncertainty reduction at the

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*Code of Federal Regulations, Title 10, Part 60 [59]

desired design life. These experiment designs are termed uncertainty-optimized (UO).

The methodology developed for this purpose couples a mechanistic multivariable model of the corrosion process, a model building database (MBD) consisting of laboratory-measured data relevant to corrosion performance of A216 steel in simulated repository brines, a model of error (uncertainty) propagation, predictions of waste container-repository in-service conditions and a collection of 'virtual' (or simulated) experiment data representing the potential experiments under evaluation for their impact on uncertainty reduction. The virtual data constitute the experiment sample space (ESS).

The above methodology required accomplishing the following major objectives in this thesis:

- Compile and characterize the repository environment as it impacts waste container degradation by corrosion
- Identification of the principle waste container corrosion mechanism and the environmental variables which affect this mechanism in repository-relevant conditions
- Assemble a database of measurements generated by the corrosion mechanism which are suitable to construct a model
- Develop a parametric model of waste container corrosion, and an algorithm to estimate the parameters based upon model building data
- Specify the expected time-dependent waste container in-service environment

- Develop an algorithm to propagate uncertainties in the time- and environment-integrated penetration

- Develop an automatic means of virtual data handling so that the virtual data is evaluated for penetration uncertainty reduction and added to the model building data in uncertainty-optimized order

5.3 ASSESSMENT OF THE MODEL

Arguments are made in Chapter 2 which justify the assumed model of failure (general corrosion) for a waste container in service. The results of high-magnesium brine static excess salt tests indicate magnesium is incorporated in the corrosion product oxide, and that this oxide is non-protective as active metal dissolution proceeds throughout the test.

The simple structure, low strength, and absolute lack of observation of microscopic (threshold) failure mechanisms for the A216 alloy provide justification for ruling out these mechanisms as a category. Caution is urged, however, in making this type of assumption for the container at the location of head-to-container joining. Weldments may lead to significantly altered microstructure and possibly large localized residual stresses. This thesis has analyzed the general corrosion attack of the A216 alloy and made the assumption that the container behaves as the alloy, ignoring design-specific features which might possibly constitute a 'weak link' to failure. This is because no detailed design information relative to final container head closure was

available at the time. The weak link potentially provided by the effects of welding are deferred to future research.

The very simple model of general corrosion for steel in magnesium-bearing brines explains all gross trends identified in the experimental data. This model has been developed largely drawing upon the consistent validity of the Arrhenius (and, more generally, the Eyring) functional form to explain chemical reaction-driven processes. The database itself has been compiled from a variety of specialized test programs. As such, unidentified, uncontrolled variables may differ from test type to test type. It is expected the fit of the model would improve greatly if a consistent database were available. At present, however, it is concluded that the corrosion rate model developed for the purpose of this thesis is entirely consistent with the available data. Largely in agreement with Peters and Kuhn [46], the kinetic behavior was found to be very nearly parabolic.

5.4 ASSESSMENT OF THE EXPERIMENT DESIGN METHODOLOGY

After extensive searching of the published literature, it was concluded that great deficiencies exist related to the explicit mathematical treatment of extrapolation. This is especially true of applied situations which involving large (factor of 10 to 100) extrapolations beyond the interval over which experimental observations have been made.

The theoretical development of a methodology to specify uncertainty-optimized experiment designs is presented in Chapter 3. Uncertainty-optimized is defined at the beginning of this thesis to mean that the product experimental design, if performed, is expected to generate data which will yield the greatest reduction in uncertainty at some desired extrapolated time value such as the design life of a waste container.

The methodology to generate uncertainty-optimized experiment designs has been developed in the form of a Fortran computer program called UNODEX (UNcertainty-Optimized DEsign of eXperiments), included as Appendix A. The UNODEX computational procedure is as follows:

1. The specified corrosion model (in general nonlinear, multivariable, and multiparameter) is fitted with maximum likelihood estimates of the unknown model parameters and errors, based solely upon the MBD.

2. The uncertainty (standard deviation) at the desired design life (300 or 1000 years) is calculated and referenced as the benchmark penetration and uncertainty.

3. Virtual data point from the ESS are sequentially evaluated, by shifting one virtual data point into the MBD, calculating the improvement in uncertainty based upon new parameter estimates (and errors), and shifting the virtual data point back out of the MBD again. This continues until each virtual data point in the ESS has an uncertainty reduction associated with it.

4. The virtual data are then cumulatively added to the MBD, in rank order, and the total reduction based on the cumulative addition is calculated at each step (*i.e.* the uncertainty reduction based on the addition of the first of the virtual data point, the first and second, the first, second and third, etc.).

5. After the ESS is evaluated cumulatively, based on the first ranking, the profile of the above uncertainty vs. number of experiments added is evaluated for the presence of a plateau, followed by a sharp discontinuity (section 4.3.5 discusses this phenomena in greater detail) and when this is found, all virtual data up to the point of the plateau are shifted into the MBD, the remaining virtual data are reevaluated sequentially as in item 3. above.

This generates the total uncertainty reduction vs. number of experiments added, in Uncertainty-Optimized (UO) order. The underlying assumptions of the UNODEX methodology and their limitations are discussed below.

First and foremost, the working hypothesis made in this work is that *The model of general corrosion developed in this thesis is structurally correct, and that it includes all the significant independent variables affecting the corrosion process.* This effectively eliminates any uncertainty due to lack of knowledge of the physical process and allows the explicit quantitative evaluation of the uncertainty (or random behavior) in the physical process itself. In fact, knowledge of the waste container corrosion process is not complete at all, and dealing with that uncertainty will necessitate, in addition to further research, the implementation of the UNODEX methodology with many different corrosion rate models.

The parameter estimates, which are determined by a maximum likelihood approach are based upon the asymptotic covariance matrix as determined

in Equation (3.43). This results from the numerically-necessary assumption of local linearity about initial guess values for the parameters. Use of the true parameter covariance matrix would prove to be mathematically intractable and frustrate convergence.

The assumption of local linearity in the parameter space is expected to prove valid, provided sufficient exploration of the parameter space is done before selecting initial guesses. This was the case for all models compared in this thesis.

The assumption was made that penetration and uncertainty in a given time interval was independent from all other time intervals. The author can think of no evidence to the contrary at the present level of corrosion model detail.

It is also assumed that the corrosion rate (dependent variable) for the virtual data under evaluation can be estimated by the model itself. This leads to simulated corrosion rate values for the ESS virtual data which lie exactly on the fitted model-predicted curve. There is no inconsistency in this procedure, as: 1) these precise values are weighted by an empirically-consistent error, and 2) only the uncertainty due to physical variability is being addressed in the thesis.

The determination of the virtual data error is a key element in the validity of the results of this work. As outlined in Section 4.3.1.2, a

simple linear regression model was formulated incorporating each of the independent variables in the corrosion rate model. As the MLE parameter estimates depend upon the weighting of the data, this same error model was used to weight the actual model building data. This approach permitted iteration between the corrosion model and the error model to determine the coefficients and parameters which were empirically-consistent.

In point of fact, the actual data included some significant outliers, which will not be the case with virtual data. In this sense the virtual data error model does not provide the worst possible error measure for the potential experiment, but it also does not provide the least. There is a smoothing effect in this determination of error, which effectively assigns the error expected for many repeated measurements.

5.5 ASSESSMENT OF THE RESULTS

Strong assumptions about the expected in-service environment are made in Section 4.3.2.1. These follow the so-called conservative approach to assessing the corrosion performance employed extensively, for example, in the Environmental Assessment for the potential Deaf Smith County Texas site*. These assumptions are:

- There is infinite reserve of high-magnesium brine available via some means of transport to the container boundary.

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*Reference [55]

- The rate of this brine availability is never the limiting step in the overall process of metal dissolution.
- The dissolved oxygen concentration in the brine is always anoxic (0.05 ppm)
- The container-salt interface is always characterized by 5 weight percent water (by brine) and 95 weight percent solid phase salt.

Based solely on the model building data, penetration and uncertainty are calculated. Results indicate 2.93 cm of uniformly penetrated container thickness at 1000 years with an uncertainty, σ of 2.11 cm, or 72%. Employing a standard 2σ confidence interval, the maximum penetration at 1000 years becomes 7.15 cm (2.81 inches).

Variations of the environmental conditions revealed a strong sensitivity to temperature, as when the commercial high level waste temperature profile was employed (9.5 kW vs. 6.6kW). Penetration and uncertainty at 1000 years became approximately 12 cm and 13 cm, respectively.

Two major techniques in interpreting the resultant uncertainty-optimized designs were implemented in the thesis: i) the 'first point' uncertainty reduction and ii) the periodic trend.

The first technique tabulates the reduction in uncertainty due to the addition of the first virtual data point to the MBD (Selected as that with maximum uncertainty reduction). Findings indicate:

1. The large uncertainty reduction associated only with this first point is due to its uniqueness relative to the model building data, as highly overstressed test conditions often provide.

2. The first point is nearly always associated with the test with all independent variables at their maximum values, that is, the most severe multivariable accelerated life test.

3. The magnitude is strongly nonlinear for varying test durations, implying, for a set of given problem constraints, significant diminishing returns exist for longer test times.

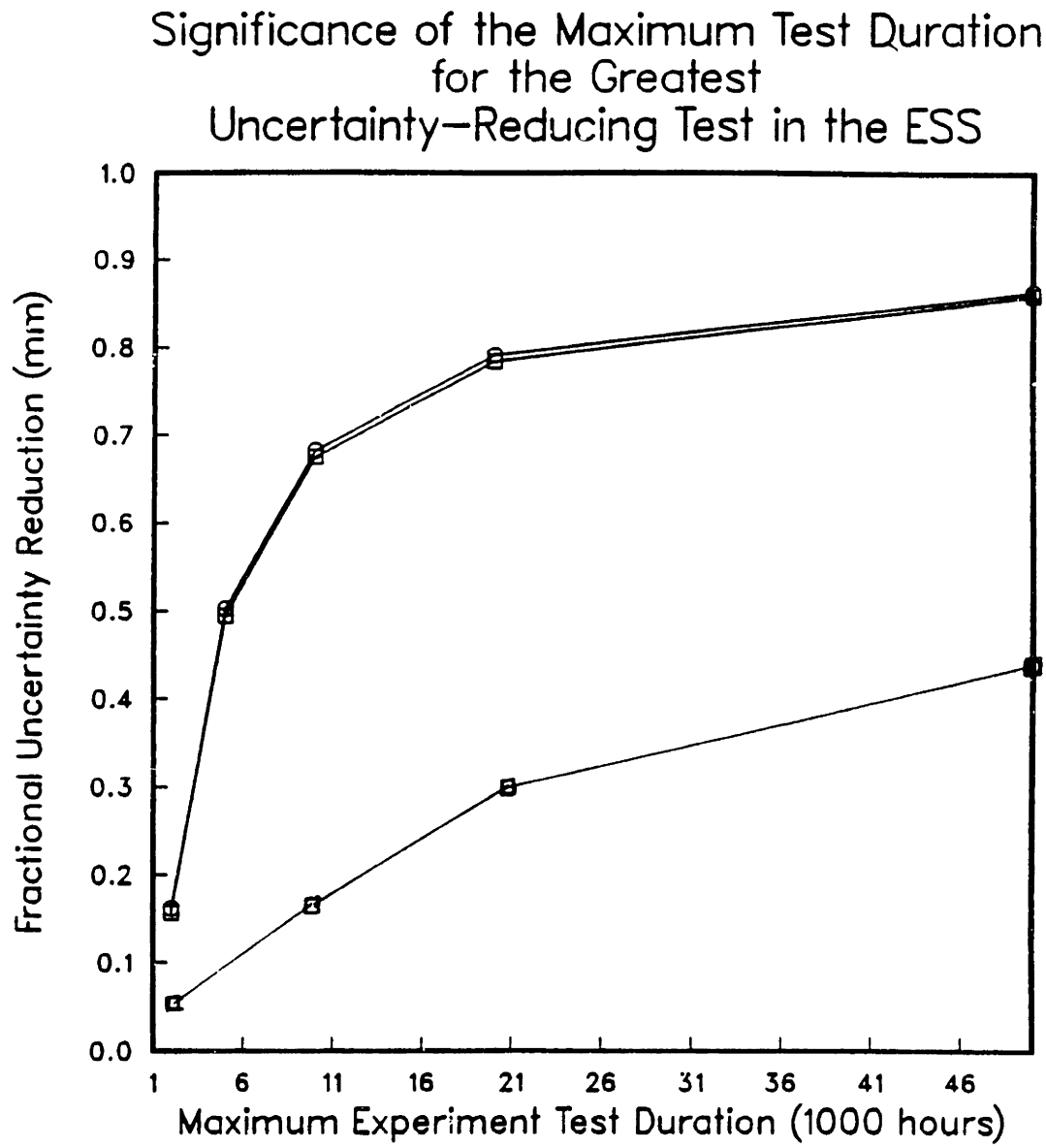
4. The magnitude is essentially linearly dependent on test temperatures, with all the other variables at their high levels.

5. When all variables are held at essentially in-service values, and time is varied, the fractional uncertainty reduction is essentially one order of magnitude lower than in the case of multivariable (all variables overstressed) accelerated life testing.

These important results are repeated here as Table 5-1.

When analyzed, it was found that the overall trend behavior for the uncertainty-optimized designs indicate a strong tendency to oscillate between repeated sequences of long- and short-term tests. This is driven by the necessity of establishing the corrosion rate vs. time behavior at the test extrema, thus enabling the most confident extrapolation.

Figure 5-1: Response of First Point Uncertainty Reduction



5.6 CONCLUSIONS

Concluding, in the context of this project - designing experiments to best meet the goal of quantitatively assessing the uncertainty of extrapolations of 1000 years - there is a very important role for both highly accelerated life testing and standard experiments conducted at essentially in-service conditions.

The later is imperative to develop the detailed corrosion process model. The former methodology is imperative, once the best model is available, to design and plan an appropriate experimental program which will provide the most effective reduction in uncertainty at the waste container design life.

The contribution and role of this new methodology, then, may be viewed as an intermediate step between lab and field data taking due to the direct incorporation of the in-service environment in the experiment design.

5.7 RECOMMENDATIONS FOR FUTURE STUDY

In order of importance, the following recommendations for future study are made.

1. A totally different problem should be analyzed, one possessing data on in-service failures, laboratory-measured short term data and a detailed, well-established process model. By this means a confirmatory exercise may be performed, providing a true test of the methodology.

2. Cost, Risk and other general functions should be developed and incorporated into the optimization variable as an option.

3. Much more diverse data should be obtained for A216 steel corrosion rate in brines to provide a better model building database.

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A. List of Acronyms

ASTM	American Society for Testing Materials
CHLW	Commercial High-Level Waste
CSF	Consolidated Spent Fuel
DHLW	Defense High-Level Waste
EA	Environmental Assessment
ESS	Experiment Sample Space
HLW	High-Level Waste
ISF	Intact Spent Fuel
MBD	Model Building Database
MCC	Materials Characterization Center
MLE	Maximum Likelihood Estimates
NACE	National Association of Corrosion Engineers
NRC	Nuclear Regulatory Commission
ORNL	Oak Ridge National Laboratory
PBB	Permian Basin Brine
PDF	Probability Distribution Function
PWR	Pressurized Water Reactor
RRC-IWG	Reference Repository Conditions Interface Working Group
SS	Stainless Steel

UNODEX	UNcertainty-Optimized Design of eXperiments
UO	Uncertainty-Optimized
USDOE	United States Department of Energy

B. Dataset Used for the Analysis of Waste Container General Corrosion

B.1 Description of the Data

The following file lists the general corrosion data used as the basis of the work. Some of the data has yet to be published. Most of the data has been published in the references authored by Westerman, et. al.

The "M" field indicates the material type, 1 coresponds to A216 Steel. The "E" field indicates an environment code, however it is completely specified in the other fields. CR is the dependent variable used throughout the work, corrosion rate. WI and WF are initial and final weights. Area is self- explanatory. T, in °C, O2 in ppm, MG in weight fraction, H2O in weight percent, and TT expressed in hours are the five independent variables, Temperature, dissolved oxygen, magnesium concentration, water fraction and test total time. TD is the down time for the test where applicable.

B.2 File Listing

182 M	E	CR	WI	WF	AREA	T	O2	MG	H2O	TD	TT	MBCOR
P530X1X	2X	20.62X	14.1605	X14.1266	X4.0782X	150X	0.05X	0.0001X	76X	41X	696X	AGC
P531X1X	2X	11.11X	14.1771	X14.0294	X4.0743X	150X	0.05X	0.0001X	76X	114X	5835X	AGC
P532X1X	2X	12.65X	14.1359	X13.9676	X4.0811X	150X	0.05X	0.0001X	76X	114X	5835X	AGC
P533X1X	2X	10.36X	14.1369	X13.9989	X4.0850X	150X	0.05X	0.0001X	76X	114X	5835X	AGC
P534X1X	2X	12.15X	14.1560	X13.9944	X4.0811X	150X	0.05X	0.0001X	76X	114X	5835X	AGC
P535X1X	2X	13.32X	14.2159	X14.0383	X4.0908X	150X	0.05X	0.0001X	76X	114X	5835X	AGC
P536X1X	2X	15.25X	14.1525	X14.0479	X4.0908X	150X	0.05X	0.0001X	76X	66X	2897X	AGC
P537X1X	2X	16.81X	14.2059	X13.9946	X4.0811X	150X	0.05X	0.0001X	76X	428X	5321X	AGC
P538X1X	2X	16.23X	14.2217	X14.0176	X4.0840X	150X	0.05X	0.0001X	76X	428X	5321X	AGC
P539X1X	2X	16.71X	14.1792	X13.9691	X4.0850X	150X	0.05X	0.0001X	76X	428X	5321X	AGC
P540X1X	2X	18.94X	14.1427	X14.1116	X4.0732X	150X	0.05X	0.0001X	76X	41X	696X	AGC
P541X1X	2X	18.45X	14.2126	X13.9308	X4.0908X	150X	0.05X	0.0001X	76X	428X	5321X	AGC
P542X1X	2X	13.09X	14.2099	X14.0452	X4.0840X	150X	0.05X	0.0001X	76X	428X	5321X	AGC
P543X1X	2X	13.02X	13.9079	X13.8190	X4.0732X	150X	0.05X	0.0001X	76X	66X	2897X	AGC
P544X1X	2X	18.88X	14.1028	X13.8657	X4.0801X	150X	0.05X	0.0001X	76X	428X	5321X	AGC
P545X1X	2X	26.53X	14.1828	X13.8553	X4.0850X	150X	1.50X	0.0001X	76X	782X	5384X	OGC
P546X1X	2X	21.74X	14.1911	X13.9147	X4.0821X	150X	1.50X	0.0001X	76X	81X	5384X	OGC
P547X1X	2X	27.60X	13.9014	X13.7125	X4.0675X	150X	1.50X	0.0001X	76X	36X	2908X	OGC
P548X1X	2X	28.18X	14.0968	X13.0477	X4.0811X	150X	1.50X	0.0001X	76X	0X	736X	OGC
P549X1X	2X	26.55X	14.1001	X13.7626	X4.0811X	150X	1.50X	0.0001X	76X	81X	5384X	OGC
P550X1X	2X	30.34X	14.1494	X13.7644	X4.0743X	150X	1.50X	0.0001X	76X	81X	5384X	OGC
P551X1X	2X	24.11X	14.2305	X13.9240	X4.0801X	150X	1.50X	0.0001X	76X	81X	5384X	OGC
P552X1X	2X	14.94X	14.2179	X14.1155	X4.0714X	150X	1.50X	0.0001X	76X	36X	2908X	OGC
P553X1X	2X	21.29X	14.0262	X13.7562	X4.0714X	150X	1.50X	0.0001X	76X	81X	5384X	OGC
P554X1X	2X	26.31X	14.1614	X14.1157	X4.0674X	150X	1.50X	0.0001X	76X	0X	736X	OGC
P555X1X	2X	23.43X	14.2017	X13.9046	X4.0703X	150X	1.50X	0.0001X	76X	81X	5384X	OGC
P556X1X	2X	21.79X	14.1989	X13.9224	X4.0742X	150X	1.50X	0.0001X	76X	81X	5384X	OGC
P557X1X	2X	28.69X	14.0682	X13.7042	X4.0732X	150X	1.50X	0.0001X	76X	81X	5384X	OGC
P515X1X	2X	29.41X	14.1927	0X14.1394	X4.1025X	150X	0.05X	0.0001X	76X	0X	768X	IC1
P516X1X	2X	16.31X	14.1614	0X14.0771	X4.1025X	150X	0.05X	0.0001X	76X	510X	2180X	IC1
P517X1X	2X	14.36X	14.0504	0X13.9149	X4.1094X	150X	0.05X	0.0001X	76X	726X	3974X	IC1
P519X1X	2X	15.44X	14.1540	0X13.9675	X4.0957X	150X	0.05X	0.0001X	76X	1405X	5099X	IC1
P520X1X	2X	11.60X	14.1655	0X14.0562	X4.1025X	150X	0.05X	0.0001X	76X	726X	3974X	IC1
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P522X1X	2X	10.23X	14.1328	0X14.0364	X4.1025X	150X	0.05X	0.0001X	76X	726X	3974X	IC1
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P653X1X	13X	488.1X	1.8463	X1.3422	X0.8198X	150X	0.05X	0.0042X	5X	0X	2178X	XS2A
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P666X1X	13X	669.4X	1.8065	X1.1176	X0.8172X	150X	0.05X	0.0170X	20X	0X	2178X	XS2C
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R979X1X53X28.82X 4.65910X 4.62345X0.9690X 90X0.05X0.0134X20X   0X 2203X ES2
Q414X1X53X489.1X 2.70570X 2.15885X0.8855X150X0.05X0.0134X20X   0X 2179X ES6
Q416X1X53X559.6X 2.73045X 2.11135X0.8762X150X0.05X0.0134X20X   0X 2179X ES6
Q422X1X53X388.3X 2.72710X 2.29680X0.8777X150X0.05X0.0134X20X   0X 2179X ES6
Q431X1X51X24.75X 2.72865X 2.70110X0.8817X150X0.05X0.0001X20X   0X 2179X ES8
Q432X1X51X20.76X 2.74635X 2.72345X0.8737X150X0.05X0.0001X20X   0X 2179X ES8
Q436X1X51X04.43X 2.71110X 2.70620X0.8764X150X0.05X0.0001X20X   0X 2179X ES8
Q452X1X51X17.69X 2.77315X 2.75365X0.8826X150X0.05X0.0001X20X   0X 2155X ES8A
Q461X1X51X25.16X 2.72560X 2.69790X0.8815X150X0.05X0.0001X20X   0X 2155X ES8A
Q469X1X51X18.86X 2.75285X 2.73240X0.8682X150X0.05X0.0001X20X   0X 2155X ES8A
Q434X1X51X07.83X 2.69855X 2.68805X0.8695X 90X0.05X0.0001X20X   0X 2155X ES10
Q435X1X51X08.78X 2.71990X 2.71040X0.8669X 90XC.05X0.0001X20X   0X 2155X ES10
Q438X1X51X08.37X 2.73365X 2.72455X0.8709X 90X0.05X0.0001X20X   0X 2155X ES10
Q455X1X51X06.33X 2.66760X 2.66070X0.8735X150X0.05X0.0001X05X   0X 2155X ES14
Q480X1X51X06.87X 2.73850X 2.73125X0.8709X150X0.05X0.0001X05X   0X 2155X ES14
Q467X1X51X08.15X 2.75780X 2.74895X0.8695X150X0.05X0.0001X05X   0X 2155X ES14
Q444X1X51X03.09X 2.74255X 2.73220X0.8695X 90X0.05X0.0001X05X   0X 2155X ES18
Q458X1X51X03.08X 2.72125X 2.71790X0.8711X 90X0.05X0.0001X05X   0X 2155X ES18
Q463X1X51X02.90X 2.72730X 2.72415X0.8695X 90X0.05X0.0001X05X   0X 2155X ES18
Q450X1X51X107.8X 2.72950X 2.61205X0.8722X200X0.05X0.0001X05X   0X 2155X ES18
Q451X1X51X89.43X 2.73365X 2.63625X0.8722X200X0.05X0.0001X05X   0X 2155X ES18
Q453X1X51X80.83X 2.74190X 2.65360X0.8748X200X0.05X0.0001X05X   0X 2155X ES18
Q472X1X53X422.0X 2.75265X 2.27415X0.8669X150X0.05X0.0034X05X   0X 2155X ES20
Q473X1X53X335.0X 2.72065X 2.35635X0.8708X150X0.05X0.0034X05X   0X 2155X ES20
```

```
Q476X1X53X320.3X 2.70940X 2.36165X0.8695X150X0.05X0.0034X05X   0X 2155X ES20
Q481X1X53X11.83X 2.74450X 2.73160X0.8735X 90X0.05X0.0034X05X   0X 2155X ES22
Q484X1X53X16.51X 2.74000X 2.72215X0.8656X 90X0.05X0.0034X05X   0X 2155X ES22
Q485X1X53X10.90X 2.72155X 2.70975X0.8671X 90X0.05X0.0034X05X   0X 2155X ES22
Q483X1X53X881.7X 2.72540X 1.77500X0.8631X200X0.05X0.0034X05X   0X 2155X ES24
Q486X1X53X883.2X 2.74365X 1.78895X0.8656X200X0.05X0.0034X05X   0X 2155X ES24
Q438X1X53X950.0X 2.71975X 1.69580X0.8631X200X0.05X0.0034X05X   0X 2155X ES24
Q690X1X53X625.9X 2.75550X 2.05810X0.8922X200X0.05X0.0034X05X   0X 2155X ES24
T 53X1X53X668.6X 2.70315X 1.98160X0.8642X200X0.05X0.0034X05X   0X 2155X ES24
```

C. THE UNODEX SYSTEM COMPUTER PROGRAM

C.1 Users Documentation

C.1.1 Input to UNODEX

Input to UNODEX consists of the following:

VARIABLE	DESCRIPTION
Card 1: Format(I4)	
IESSNO	Problem Identifier Number
Card 2: Format(I4)	
NTLNS	Number of Title Lines Following
Card(s) 3: Format(NTLNS*A60)	
TITLE(1)	Title Cards
TITLE(NTLNS)	
Card 4: Format(I4)	
NIV	Number of Independent Variables
Card(s) 5: Format(NIV(A12,2F10.5,I5))	
NAME(1),XH(1),XL(1),NLEV(1)	Name of IV, high level, low level and number of levels the IV is to assume in the generation of the experiment sample space.

NAME(NIV),XH(NIV),XL(NIVH),NLEV(NIV)

Card 6: Format(19I4,4E10.1)

CNTROL(1) Number (of total number) of parameters to be fitted

CNTROL(2) Total number parameters

CNTROL(3) Number of data points

CNTROL(4) Dimensions of the A-array and 1st dimension of the B-array, must be at least the largest value of CNTROL(2)

CNTROL(5) Total number variables (1 dependent + any number of independent)

CNTROL(6) Limit on number of iterations

CNTROL(7) Print control
= 0: no intermediate output wanted
= +1: Print input data
= +2: Print sum of squares and parameter values
= +4: Print normal equations
= +8: Print restrained change mechanism
=+16: Print point-by-point comparison

CNTROL(8) Index identifying the weighting function for the sum of squares
= 1: 1.0
= 2: 1/OBS
= 3: 1/CALC
= 4: OBS
= 5: CALC
= 6: 1/Z(C5,N), Z(C5,N) = ERROR IN OBS VAL OF Y

= 7: Z(C5,N)
= 8: 1/MX(O,C) = Inverse of the maximum of the observed and the calculated values

CNTROL(9) Convergence criteria control

CNTROL(10) Parameter variation constraint for restrained change mechanism
= 0: Unconstrained parameter changes
> 0: Limit on percentage change of parameter expressed in units in tens of percent

CNTROL(11) Controlfor overriding the restrained change mechanism
=1: Overriding permitted, unconstrained changes in the parameters are permitted
=0: No overriding

CNTROL(12) Control for overriding sum of square reduction test
=Number of overrides permitted per iteration

CNTROL(13) Parameter change option

CNTROL(14) NOT USED

CNTROL(15) Derivative specification control
= 1: Analytic derivative provided in a user-defined function called DYDB.FOR
= 0: No Derivative function provided, calculate derivatives numerically

CNTROL(16) Total number of problems to be solved

CNTROL(17) Number of sets of guesses

CNTROL(18) Number of different dependent variable expressions prepared in YO.FOR

CNTROL(19) Y Index identifying which (of multiple) expression(s) for YO to use

SCONVG Cauchy convergence on error sum of squares

PCONVG	Cauchy convergence on parameters
BCONVG	Cauchy convergence on individual parameter
ADEL	Convergence on detection of plateau in uncertainty reduction vs experiment number.

Card 7: Format(2I4)

NTIMES	Number of timesteps for error propagation routine
IDLIFE	The timestep at which the uncertainty is minimized

Card(s) 8: Format(NIV*(NTIMES*E10.5))

XINSERV(I,J),I=1,NIV, J=1,NTIMES
Values for the in-service environmental boundary conditions.

Card 9: Format(2I5,CNTROL(1)*E11.4)

IB,IC,BTRIAL(I),I=1,CNTROL(1)
Total number of parameters, number to be fitted this trial and trial values (initial guesses) for the parameters

---

C.1.1.1 Sample Problem Input Deck

JOB.DAT

```
201
  3
WASTE CONTAINER PENETRATION UNCERTAINTY
    2**5 REF MATRIX, 300 YEAR
        20,000 HR MAX TIME
   5
TEMP          220.0          80.0          2
[ O2 ]          2.0          0.05          2
[ Mg ]         0.06          .001          2
WT % H2O       80.0           5.0          2
TIME (hr)   20000.0         750.0          2
  3  3 40  4  8 70  0  0  8  1  4  0  2  0  0  1  1  1  1  1  5.0E-07  1.0E-05  1.0E-02  2.0E-01
 11  9
 1.348E+2  1.349E+2  1.344E+2  1.307E+2  1.245E+2  1.067E+2  8.94E+1  7.53E+1  7.20E+1  6.81E+1  5.99E+1    TEMP
   5.0E-2    5.0E-2    5.0E-2    5.0E-2    5.0E-2    5.0E-2   5.0E-2   5.0E-2   5.0E-2   5.0E-2   5.0E-2    [O2]
   5.0E-2    5.0E-2    5.0E-2    5.0E-2    5.0E-2    5.0E-2   5.0E-2   5.0E-2   5.0E-2   5.0E-2   5.0E-2    [MG]
   5.0E+0    5.0E+0    5.0E+0    5.0E+0    5.0E+0    5.0E+0   5.0E+0   5.0E+0   5.0E+0   5.0E+0   5.0E+0   %H2O
   1.0E+0    2.0E+0    5.0E+0    1.0E+1    2.0E+1    5.0E+1   1.0E+2   2.0E+2   3.0E+2   5.0E+2   1.0E+3    TIME
   3    3 2.3500E+11  1450.0000   1.81e+04    0.00001    0.600000 5793.0
12345678901234567890123456789012345678901234567890123456789012345678901234567890
  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19    SCONVG    PCONVG    BCONVG
```

C.2 Program Source Listing

```
      PROGRAM UNODEX                                                    UNODEX
C ***********************************************************************UNODEX
C *                                                                     *UNODEX
C *                                                                     *UNODEX
C *    The UNODEX Program                          September 1986       *UNODEX
C *                                                                     *UNODEX
C *        UNcertainty Optimized Design of EXperiments                  *UNODEX
C *                                                                     *UNODEX
C *                                                                     *UNODEX
C *        By      A. J. Wolford                                        *UNODEX
C *                Department of Nuclear Engineering                    *UNODEX
C *                Massachusetts Institute of Technology                *UNODEX
C *                Developed in partial fulfillment of his ScD          *UNODEX
C *                at, and with thanks to                               *UNODEX
C *                The Battelle Memorial Institute                      *UNODEX
C *                Columbus, Ohio                                       *UNODEX
C *                                                                     *UNODEX
C *                and                                                  *UNODEX
C *                                                                     *UNODEX
C *                R. A. Christensen                                    *UNODEX
C *                R. F. Eilbert                                        *UNODEX
C *                Entropy, Ltd.                                        *UNODEX
C *                Lincoln, Massachusetts                               *UNODEX
C *                                                                     *UNODEX
C *                                                                     *UNODEX
C *                Original version FITSALL algorithm credits:          *UNODEX
C *                                                                     *UNODEX
C *                by R. A. Christensen, T. A. Reichert, and others     *UNODEX
C *                Physics and Chemistry Depts.                         *UNODEX
C *                University of California, Berkeley                   *UNODEX
C *                1968-1969                                            *UNODEX
C *                                                                     *UNODEX
C ***********************************************************************UNODEX
C ***********************************************************************UNODEX
C *                              EXAMPLE:                               *UNODEX
C ***********************************************************************UNODEX
C                                                                       UNODEX
C       Y(N) = ( B(1) + B(2)*X(1,N) ) * EXP( -B(3)/X(2,N) )             UNODEX
C                                                                       UNODEX
C       B(J) = J-TH PARAMETER TO BE FITTED                              UNODEX
C       X(I,N) = OBSERVED VALUE OF I-TH INDEP VARIABLE FOR N-TH DATA PT UNODEX
C       Y(N) = OBSERVED VALUE OF DEPENDENT VARIABLE FOR N-TH DATA POINT UNODEX
C                                                                       UNODEX
C    (FITSALL IS ABLE TO LOOP OVER DIFFERENT FUNCT. FORMS FOR Y(N))     UNODEX
C                                                                       UNODEX
C ***********************************************************************UNODEX
C *               INPUT READ ON LOGICAL UNIT 12:                       *UNODEX
C ***********************************************************************UNODEX
C.. ALL CNTROL(1,24) ARE VIA COMMON/CNTROL                              UNODEX
C                                                                       UNODEX
C                                                                       UNODEX
C                                                                       UNODEX
C       CNTROL(1)=NB (NUMBER OF B'S): NUMBER (OF TOTAL NUMBER) OF       UNODEX
C                     PARAMETERS TO BE FITTED                           UNODEX
C                                                                       UNODEX
C       CNTROL(2)=M3: TOTAL # PARAMETERS                                UNODEX
C                                                                       UNODEX
C       CNTROL(3)=-INT3: NUMBER DATA POINTS                             UNODEX
```

```
C          BDIM=CNTROL(4)=DIMS OF A-ARRAY & 1ST DIM OF B-ARRAY,          UNODEX
C          MUST BE AT LEAST THE LARGEST VALUE OF CNTROL(2)               UNODEX
C                                                                        UNODEX
C       CNTROL(5)=NVARS: TOTAL NUMBER VARIABLES                          UNODEX
C             (1 DEPENDENT + ANY NUMBER OF INDEPENDENT)                  UNODEX
C                                                                        UNODEX
C       CNTROL(6)=LIMIT: LIMIT ON # INTERATIONS                          UNODEX
C                                                                        UNODEX
C       CNTROL(7): PRINT CONTROL                                         UNODEX
C                =  0: NO INTERMEDIATE OUTPUT WANTED                     UNODEX
C                = +1: PRINT INPUT DATA                                  UNODEX
C                = +2: PRINT SUMSQ & PARM VALS                           UNODEX
C                = +4: PRINT NORMAL EQUATIONS                            UNODEX
C                = +8: PRINT RESTRAINED CHANGE MECHANISM                 UNODEX
C                =+16: PRINT POINT-BY-POINT COMPARISON                   UNODEX
C                                                                        UNODEX
C       CNTROL(8)=LL: INDEX IDENTIFYING WEIGHTING FCN FOR SSQ            UNODEX
C                = 1: 1.0                                                UNODEX
C                = 2: 1/OBS                                              UNODEX
C                = 3: 1/CALC                                             UNODEX
C                = 4: OBS                                                UNODEX
C                = 5: CALC                                               UNODEX
C                = 6: 1/Z(C5,N), Z(C5,N) = ERROR IN OBS VAL OF Y         UNODEX
C                = 7: Z(C5,N)                                            UNODEX
C                = 8: 1/MX(0,C) [...INVERSE OF MAX OF OBS & CALC VALS]   UNODEX
C                                                                        UNODEX
C       CNTROL(9)=CONVERGENCE CRITERIA CONTROL                           UNODEX
C                 = 1:                                                   UNODEX
C                 = 2:                                                   UNODEX
C          TO BTEST -- IT SWITCHES FROM PCONVG TO BCONVG]                UNODEX
C                                                                        UNODEX
C       CNTROL(10)=KNTR10:  RESTRAINED CHANGE MECHANISM: PARAMETER       UNODEX
C                           VARIATION CONSTRAINT IN TENS OF PERCENT      UNODEX
C                 = 0: UNCONSTRAINED PARAMETER CHANGES                   UNODEX
C                 > 0: LIMIT ON PERCENTAGE CHANGE OF PARAMETERS          UNODEX
C                      [EXPRESSED IN UNITS OF TENS OF PERCENT]           UNODEX
C                                                                        UNODEX
C       CNTROL(11)=CONTROL FOR OVERRIDING RESTRAINED CHANGE MECHANISM    UNODEX
C                 =1: OVERRIDING PERMITTED                               UNODEX
C                    (UNCONSTRAINED CHANGES ALLOWED WHEN OVERRIDDEN)     UNODEX
C                 =0: NO OVERRIDING                                      UNODEX
C                                                                        UNODEX
C       CNTROL(12)=CONTROL FOR OVERRIDING SSQ REDUCTION TEST             UNODEX
C                 =NUMBER OF OVERRIDES PERMITTED                         UNODEX
C                  (NEGATIVE VALUE ACTIVATES WRONG WAY MECHANISM)        UNODEX
C                                                                        UNODEX
C       CNTROL(13)= ?? (PARAMETER CHANGE OPTION ?)                       UNODEX
C                                                                        UNODEX
C       CNTROL(14)=[NOT USED]                                            UNODEX
C                                                                        UNODEX
C       CNTROL(15)=DERIVATIVE CONTROL                                    UNODEX
C                 = 1: ANALYTIC DERIVATIVE PROVIDED IN A FN NAMED DYDB   UNODEX
C                 = 0: NOT PROVIDED, NUMERICAL DERIVS WILL BE COMPUTED   UNODEX
C                                                                        UNODEX
C       CNTROL(16)=TOTAL NUMBER OF PROBLEMS TO BE SOLVED                 UNODEX
C                                                                        UNODEX
C       CNTROL(17)=NSETS=NUMBER OF SETS OF GUESSES                       UNODEX
C                                                                        UNODEX
```

```
C       CNTROL(18)=NUMBER OF DIFFERENT DV EXPRESSIONS PREPARED IN YO    UNODEX
C                                                                       UNODEX
C       CNTROL(19)=Y INDEX (TO LET YCOMP.FR & DERIV.FR KNOW WHICH       UNODEX
C              EXPRESSION TO USE OF Y) (MUST NOT EXCEED CNTROL(18))     UNODEX
C                                                                       UNODEX
C       CNTROL(20)=NN:  NUMBER OF ITERATIONS USED                       UNODEX
C                                                                       UNODEX
C       CNTROL(21)=IHOLD:  TERMINATION CODE                             UNODEX
C                 =0: OPTION REDUNDANCY, EXPRESSION CHG INDICATED       UNODEX
C                 =1: CAUCHY CONVERGENCE OF PARAMETERS                  UNODEX
C                 =2: CAUCHY CONVERGENCE OF SUM OF SQUARES              UNODEX
C                 =3: HIT LIMIT ON # ITERATIONS                         UNODEX
C                 =4: EQNS SINGULAR                                     UNODEX
C                 =5: NO SSQ REDUCTION - GUESS AGAIN                    UNODEX
C                                                                       UNODEX
C       CNTROL(22)=INITIAL ENTRY FLAG                                   UNODEX
C                 =1: INITIAL ENTRY TO GAUSS.FR; IN YCOMP.FR,           UNODEX
C                              SET Z(   ,   ) = OBSERVED VALUES         UNODEX
C                 =0: SUBSEQUENT ENTRY; IN YCOMP.FR COMPUTE VALUE OF Y  UNODEX
C                                                                       UNODEX
C       CNTROL(23)=II:  SEQUENCE # OF PROBLEM BEING PROCESSED           UNODEX
C                                       [MAX IS CNTROL(16)]             UNODEX
C                                                                       UNODEX
C       CNTROL(24)=K: SEQUENCE # OF GUESS SET BEING PROCESSED           UNODEX
C                                                                       UNODEX
C       CNTROL(25)= [NOT USED]                                          UNODEX
C                                                                       UNODEX
C       IB=TOTAL # PARAMETERS THIS TRIAL                                UNODEX
C                                                                       UNODEX
C       IC=# PARAMETERS TO BE FITTED THIS TRIAL                         UNODEX
C                                                                       UNODEX
C       BTRIAL(1,...,IB)=INITIAL GUESS OF PARAMETER VALUES              UNODEX
C                                                                       UNODEX
C ***********************************************************************UNODEX
C *                      DEFINITIONS AND COMMENTS                       *UNODEX
C ***********************************************************************UNODEX
C                                                                       UNODEX
C       NDIM=2ND DIMENSION OF Z(   ,   ), MUST BE AT LEAST NPTS         UNODEX
C            NPTS=IABS(CNTROL(3))=# DATA POINTS                         UNODEX
C            (NEGATIVE VALUE INDICATES INITAL ENTRY FOR                 UNODEX
C            PRELIMINARY CALLS TO YCOMP.FR AND GAUSS.FR)                UNODEX
C                                                                       UNODEX
C       MDIM=1ST DIMENSION OF Z(   ,   )                                UNODEX
C            MDIM                                                       UNODEX
C               =VARS.....[USUALLY]                                     UNODEX
C               =VARS+1...[IF CNTROL(8)=6 OR 7,TO GIVE ROOM FOR ERR     UNODEX
C                                                                       UNODEX
C       IBCHN                                                           UNODEX
C                                                                       UNODEX
C       L=TRIAL SEQUENCE #                                              UNODEX
C                                                                       UNODEX
C       NLAB=NUMBER OF LAB DATA POINTS                                  UNODEX
C                                                                       UNODEX
C       NPARAM=DIMENSION OF PARAM(   ),                                 UNODEX
C            (..MUST BE AT LEAST THE LARGEST VALUE OF CNTROL(2))        UNODEX
C                                                                       UNODEX
C       NVIR=NUMBER OF VIRTUAL DATA POINTS                              UNODEX
C                                                                       UNODEX
```

```
C ************************************************************************UNODEX
C *                      LOGICAL UNITS/CHANNEL USEAGE                    *UNODEX
C ************************************************************************UNODEX
C                                                                         UNODEX
C                                                                         UNODEX
C.......CHANNEL USAGE:                                                   UNODEX
C                                                                         UNODEX
C                                                                         UNODEX
C       CHANNEL 1:  MODEL BUILDING DATA (MBCOR.DAT)                       UNODEX
C                                                                         UNODEX
C       CHANNEL 2: EXPLANATORY OUTPUT (USER.OUT)                          UNODEX
C                                                                         UNODEX
C       CHANNEL 3: VIRTUAL (HYPOTHETICAL EXPERIMENT) INDEPENDENT          UNODEX
C                  VARIABLE DATA, GENERATED BY GENVIRT.FOR                UNODEX
C                            (VIRCOR.DAT)                                 UNODEX
C                                                                         UNODEX
C       CHANNEL 4:  B-PARAMETER INIOTIAL 'GUESS' VALUES (BTRIAL.DAT)      UNODEX
C                                                                         UNODEX
C       CHANNEL 8:  ECHELON UNCERTAINTY EVALUATION   (DELTAS.DAT)         UNODEX
C                                                                         UNODEX
C       CHANNEL 12:  PROBLEM INPUT CONTROL DECK   (JOB.DAT)               UNODEX
C                                                                         UNODEX
C                                                                         UNODEX
C************************************************************************UNODEX
C************************************************************************UNODEX
        PARAMETER NDTS=1250                                               UNODEX
        PARAMETER NVMAX=1250                                              UNODEX
        COMMON X(8,NDTS),Y(1,NDTS),E(1,NDTS) !;MAKE CONSIST WITH YCOMP    UNODEX
        DIMENSION PARAM(10),AC(100)                                       UNODEX
        DIMENSION XH(10), XL(10), NLEV(10)                                UNODEX
        DIMENSION TEMP(NVMAX)                                             UNODEX
        INTEGER LT(NVMAX), UT(NVMAX)                                      UNODEX
        INTEGER CNTROL                                                    UNODEX
        INTEGER NTLNS,NIV,NTIMES                                          UNODEX
        CHARACTER*80 TITLE                                                UNODEX
        CHARACTER*12 NAME(10)                                             UNODEX
        CHARACTER*8 TOD                                                   UNODEX
        CHARACTER*9 MDY                                                   UNODEX
        COMMON/IESS/IESSNO                                                UNODEX
        COMMON/TITLE/TITLE(5)                                             UNODEX
        COMMON/CNTROL/CNTROL(25)                                          UNODEX
        COMMON/CONVG/SCONVG,PCONVG,BCONVG                                 UNODEX
        COMMON/XINSERV/XINSERV(5,11), SIGREF(11)                          UNODEX
        COMMON/LABEL/LLAB(2)                                              UNODEX
        COMMON/XV/XVIR(5,NVMAX),IVIR(NVMAX),LVIR(2,NVMAX),                UNODEX
     +             DS(NVMAX),DDS(NVMAX),YVIR(NVMAX)                      UNODEX
                                                                          UNODEX
C.. OPEN LOGICAL UNITS                                                    UNODEX
                                                                          UNODEX
C.. CHANNEL 1 >> MBCOR.DAT: LAB DATA (INPUT RAW DATA)                     UNODEX
        OPEN (UNIT=1,FILE='MBCOR.DAT',STATUS='OLD')                       UNODEX
C       CALL FOPEN(1,'MBCOR1.DT')                                         UNODEX
                                                                          UNODEX
C.. CHANNEL 2 >> USER.OUT: EXPLANATORY OUTPUT                             UNODEX
        OPEN (UNIT=2,FILE='USER.OUT',STATUS='NEW',                        UNODEX
     +         CARRIAGECONTROL='LIST')                                   UNODEX
                                                                          UNODEX
C.. CHANNEL 3 >> VIRCOR.DAT: VIRTUAL (HYPOTHETICAL EXPERIMENT) IV DATA    UNODEX
```

```
      OPEN (UNIT=3,FILE='VIRCOR.DAT',STATUS='NEW',                    UNODEX
     +      CARRIAGECONTROL='LIST')                                    UNODEX
                                                                       UNODEX
C.. CHANNEL 4 >> BTRIAL.DAT: B PARAMETER TRIAL GUESSES                 UNODEX
      OPEN (UNIT=4,FILE='BTRIAL.DAT',STATUS='NEW',                     UNODEX
     +      CARRIAGECONTROL='LIST')                                    UNODEX
                                                                       UNODEX
C.. CHANNEL 6 >> CONSOLE.OUT: NORMAL SYS$OUT OUTPUT                    UNODEX
C      OPEN (UNIT=6,FILE='CONSOLE.OUT',STATUS='NEW',                   UNODEX
                                                                       UNODEX
C.. CHANNEL 8 >> DS.DAT: UNCERTAINTY IMPROVEMENT DATA                  UNODEX
      OPEN (UNIT=8,FILE='DS.DAT',STATUS='NEW',CARRIAGECONTROL='LIST')UNODEX
C     +      CARRIAGECONTROL='LIST')                                  UNODEX
                                                                       UNODEX
C.. CHANNEL 9 >> FOUT.DAT: ERROR MATRIX                               UNODEX
      OPEN (UNIT=9,FILE='FOUT',STATUS='NEW',CARRIAGECONTROL='LIST')    UNODEX
                                                                       UNODEX
C.. CHANNEL 12 >> JOB.DAT: PROBLEM INPUT CONTROL DECK                  UNODEX
C      OPEN (UNIT=12,FILE='JOB.DAT',STATUS='OLD',                      UNODEX
C     +      CARRIAGECONTROL='LIST')                                  UNODEX
                                                                       UNODEX
C*********************************************************************UNODEX
C*                    BEGIN INITIALIZATION                           *UNODEX
C*********************************************************************UNODEX
C.. READ IN PROBLEM TITLE FROM PRIMARY JOB CONTROL FILE                UNODEX
                                                                       UNODEX
C.. IESSNO=EXPERIMENT SAMPLE SPACE NUMBER, OR MAY BE USED              UNODEX
C   IN GENERAL AS A PROBLEM IDENTIFIER NUMBER                          UNODEX
                                                                       UNODEX
      READ(12,81)IESSNO                                                UNODEX
      WRITE(6,81)IESSNO                                                UNODEX
                                                                       UNODEX
C.. NTLINES=NUMBER OF DESCRIPTIVE PROBLEM TITLE LINES FOLLOWING        UNODEX
C   MAXIMUM IS 5                                                       UNODEX
                                                                       UNODEX
      READ(12,81)NTLNS                                                 UNODEX
   81 FORMAT(I4)                                                       UNODEX
      WRITE(6,81)NTLNS                                                 UNODEX
      READ(12,83) (TITLE(IT),IT=1,NTLNS)                               UNODEX
   83 FORMAT(A80)                                                      UNODEX
      WRITE(6,83) (TITLE(IT),IT=1,NTLNS)                               UNODEX
                                                                       UNODEX
      CALL DATE(MDY)                                                   UNODEX
      CALL TIME(TOD)                                                   UNODEX
      WRITE(2,101)TITLE(1),MDY,TOD                                     UNODEX
  101 FORMAT(10X,' UNODEX  V1.0:      ',15X,A80,4X,A9,'  ',A8)         UNODEX
      WRITE(2,85) (TITLE(ITITL),ITITL=2,NTLNS)                         UNODEX
   85 FORMAT(4(44X,A80,/)///)                                          UNODEX
      WRITE(2,80) IESSNO                                               UNODEX
   80 FORMAT(50X,'EVALUATION OF ESS ',I5)                              UNODEX
      WRITE(2,30)                                                      UNODEX
   30 FORMAT(///,'*****************************************',/,       UNODEX
     +           '* BEGIN INPUT PROBLEM AND JOB CONTROL DATA *',/,    UNODEX
     +           '*****************************************',///)     UNODEX
                                                                       UNODEX
C.. READ IN GENVIRT SETUP DATA FROM PRIMARY JOB CONTROL FILE           UNODEX
                                                                       UNODEX
      READ(12,81)NIV                                                   UNODEX
```

```
      WRITE(6,81)NIV                                                    UNODEX
                                                                        UNODEX
      READ(12,984) (NAME(KG),XH(KG),XL(KG),NLEV(KG),KG=1,NIV)           UNODEX
      WRITE(6,840) (NAME(KG),XH(KG),XL(KG),NLEV(KG),KG=1,NIV)           UNODEX
  984 FORMAT(A12,2F10.5,I5)                                             UNODEX
  840 FORMAT(A12,2E12.5,I5)                                             UNODEX
                                                                        UNODEX
C.. READ IN CONTROL VARIABLES FROM PRIMARY JOB CONTROL FILE             UNODEX
                                                                        UNODEX
      READ(12,1) (CNTROL(I),I=1,19),SCONVG,PCONVG,BCONVG,ADEL           UNODEX
      WRITE(6,1) (CNTROL(I),I=1,19),SCONVG,PCONVG,BCONVG,ADEL           UNODEX
    1 FORMAT(19I4,4E10.1)                                               UNODEX
      NPARAM=CNTROL(2)                                                  UNODEX
      NVARS=CNTROL(5)                                                   UNODEX
      IF (NIV.NE.(NVARS-1)) WRITE(6,*)'INPUT DATA ERROR, CHECK NIV'     UNODEX
      NIV=NVARS-1                                                       UNODEX
      IF(CNTROL(18).LE.0)CNTROL(18)=1                                   UNODEX
                                                                        UNODEX
                                                                        UNODEX
C.. READ IN PROJECTIONS OF EXPECTED IN-SERVICE ENVIRONMENT              UNODEX
C   FOR ALL INDEPENDENT VARIABLES                                       UNODEX
                                                                        UNODEX
      READ(12,77) NTIMES, IDLIFE                                        UNODEX
      WRITE(6,77) NTIMES, IDLIFE                                        UNODEX
   77 FORMAT(2I4)                                                       UNODEX
      DO 51 ISV=1,NIV                                                   UNODEX
      READ(12,850) (XINSERV(ISV,JSV),JSV=1,NTIMES)                      UNODEX
      WRITE(6,850) (XINSERV(ISV,JSV),JSV=1,NTIMES)                      UNODEX
  850 FORMAT(13E10.5)                                                   UNODEX
   51 CONTINUE                                                          UNODEX
                                                                        UNODEX
C.. GENERATE VIRTUAL IV DATA                                            UNODEX
                                                                        UNODEX
      CALL GENVIRT(NAME,NIV,XH,XL,NLEV,NVIR)                            UNODEX
      WRITE(6,*)'NVIR=',NVIR                                            UNODEX
D     WRITE(6,990)                                                      UNODEX
  990 FORMAT(/,1X,'RETURNED FROM MODULE GENVIRT')                       UNODEX
      REWIND 3                                                          UNODEX
                                                                        UNODEX
C.. READ LAB DATA (IV'S AND DV)                                         UNODEX
                                                                        UNODEX
      CALL BWRITE(NLAB)                                                 UNODEX
D     WRITE(6,991)                                                      UNODEX
  991 FORMAT(/,1X,'RETURNED FROM MODULE BWRITE')                        UNODEX
                                                                        UNODEX
      DO 5 I=1,NLAB                                                     UNODEX
      IF(CNTROL(19).EQ.2) Y(1,I)=ALOG(Y(1,I))                           UNODEX
      E(1,I)=ERE(X(1,I))                                                UNODEX
C      WRITE(6,*)'  E(1,I)=',E(1,I)                                     UNODEX
    5 CONTINUE                                                          UNODEX
                                                                        UNODEX
C.. HAVE FITSALL.FOR READ ITS VERY FIRST GUESSES FROM CHANNEL #12       UNODEX
C   IBCHN=INPUT B (PARAMETERS) CHANNEL, THIS CHANNEL MUST BE SET        UNODEX
C   BEFORE LINE 2222                                                    UNODEX
                                                                        UNODEX
      IBCHN=12                                                          UNODEX
      JTOT=0                                                            UNODEX
      JADD=0                                                            UNODEX
```

```
 2222     NLAB=NLAB+JADD                                                  UNODEX
          NVIROLD=NVIR                                                    UNODEX
          NVIR=NVIR-JADD                                                  UNODEX
                                                                          UNODEX
          IF(JADD.EQ.0)GOTO 3333                                          UNODEX
          DO 2266 K=1,2                                                   UNODEX
          DO 2233 JJ=1,NVIROLD                                            UNODEX
 2233     TEMP(JJ)=LVIR(K,JJ)                                             UNODEX
          DO 2255 JJ=1,NVIR                                               UNODEX
          J=IVIR(JJ+JADD)                                                 UNODEX
          LVIR(K,JJ)=TEMP(J)                                              UNODEX
 2255     CONTINUE                                                        UNODEX
 2266     CONTINUE                                                        UNODEX
          DO 2288 K=1,5                                                   UNODEX
          DO 2234 JJ=1,NVIROLD                                            UNODEX
 2234     TEMP(JJ)=XVIR(K,JJ)                                             UNODEX
          DO 2256 JJ=1,NVIR                                               UNODEX
          J=IVIR(JJ+JADD)                                                 UNODEX
          XVIR(K,JJ)=TEMP(J)                                              UNODEX
 2256     CONTINUE                                                        UNODEX
 2288     CONTINUE                                                        UNODEX
          DO 2299 JJ=1,NVIR                                               UNODEX
 2299     IVIR(JJ)=JJ                                                     UNODEX
 3333     CONTINUE                                                        UNODEX
          WRITE(6,*)'* * * * * * * * * * * * * * * * * * * * * *'         UNODEX
          WRITE(6,*)'          JADD = ',JADD                              UNODEX
          WRITE(6,*)'* * * * * * * * * * * * * * * * * * * * * *'         UNODEX
          WRITE(2,*)'* * * * * * * * * * * * * * * * * * * * * *'         UNODEX
          WRITE(2,*)'          JADD = ',JADD                              UNODEX
          WRITE(2,*)'* * * * * * * * * * * * * * * * * * * * * *'         UNODEX
                                                                          UNODEX
          CNTROL(3)=NLAB                                                  UNODEX
          INT3=CNTROL(3)                                                  UNODEX
                                                                          UNODEX
                                                                          UNODEX
       CALL FITSALL(INT3,PARAM,NPARAM,AC,SUMC,IBCHN,NTLNS)                UNODEX
D         WRITE(6,992)                                                    UNODEX
  992     FORMAT(/,1X,'RETURNED FROM FITSALL INITIALIZATION PASS')        UNODEX
                                                                          UNODEX
C.. INCREASE NUMBER OF POINTS BY ONE                                      UNODEX
          CNTROL(3)=NLAB+1                                                UNODEX
          INT3=CNTROL(3)                                                  UNODEX
                                                                          UNODEX
C.. LOAD THE SUBSEQUENT GUESSES FILE WITH THE RESULTS OF                  UNODEX
C    THE INITIALIZATION PASS RUN ON MODEL BUILDING DATA                   UNODEX
                                                                          UNODEX
          NB=CNTROL(1)                                                    UNODEX
          M3=CNTROL(2)                                                    UNODEX
          WRITE(4,40)M3,NB,(PARAM(I),I=1,M3)                              UNODEX
    40    FORMAT(2I5,7E11.4,(/,1X,8E10.4))                                UNODEX
          REWIND 4                                                        UNODEX
                                                                          UNODEX
C.. HAVE FITSALL READ ITS GUESSES FROM CHANNEL #4 FROM NOW ON             UNODEX
          IBCHN=4                                                         UNODEX
          IPHASE=1                                                        UNODEX
          IOUTER=0                                                        UNODEX
                                                                          UNODEX
C.. COMPUTE THE REFERENCE PENETRATION AND UNCERTAINTY BASED ON            UNODEX
```

```
C   MODEL BUILDING DATA ONLY.  THESE REFERENCE VALUES ARE USED          UNODEX
C   TO MEASURE SUBSEQUENT IMPROVEMENT VIA ADDITIONAL DATA               UNODEX
                                                                        UNODEX
      CALL ERPROP(PARAM,NPARAM,AC,SUMC,NB,NIV,CNTROL(19),               UNODEX
     +           CNTROL(3),IOUTER,IPHASE,NTIMES,IDLIFE)                UNODEX
D        WRITE(6,981)                                                   UNODEX
  981    FORMAT(/,1X,'RETURNED FROM ERPROP INITIALIZATION PASS')        UNODEX
                                                                        UNODEX
C***********************************************************************UNODEX
C*       INITIALIZATION COMPLETE    BEGIN SEQUENTIAL EVALUATION        *UNODEX
C***********************************************************************UNODEX
                                                                        UNODEX
C.. SET CALCULATION SEQUENCE FLAG (IPHASE) TO 2 INDICATING SEQUENTIAL   UNODEX
C   EVALUATION BEGINNING.  ASSIGN SCRATCH DEVICE LOGICAL UNIT NUMBER    UNODEX
C                                                                       UNODEX
        IPHASE=2                                                        UNODEX
        IVCHN=3                                                         UNODEX
C.. LOOP OVER VIRTUAL DATA POINTS                                       UNODEX
C        READ(IVCHN,490)NVIR                                            UNODEX
  490   FORMAT(I4)                                                      UNODEX
  301   DO 50 IOUTER=1,NVIR                                             UNODEX
        WRITE(6,3)IOUTER                                                UNODEX
        WRITE(2,3)IOUTER                                                UNODEX
    3   FORMAT(//,1X,'PHASE 2 ** EVALUATING EXPERIMENT NUMBER: ',I5)    UNODEX
                                                                        UNODEX
C.. APPEND NEXT VIRTUAL DATA POINT TO END OF DATA MATRIX                UNODEX
      CALL ADVIRT(IOUTER,NLAB,X(1,INT3),Y(1,INT3),E(1,INT3),            UNODEX
     +            PARAM,NPARAM,NIV)                                     UNODEX
D        WRITE(6,993)                                                   UNODEX
  993   FORMAT(/,1X,'RETURNED FROM MODULE ADVIRT')                      UNODEX
                                                                        UNODEX
      CALL FITSALL(INT3,PARAM,NPARAM,AC,SUMC,IBCHN,NTLNS)               UNODEX
D        WRITE(6,994)                                                   UNODEX
  994   FORMAT(/,1X,'RETURNED FROM MODULE FITSALL')                     UNODEX
                                                                        UNODEX
C.. COMPUTE ERROR PROPAGATION                                           UNODEX
      CALL ERPROP(PARAM,NPARAM,AC,SUMC,NB,NIV,CNTROL(19),               UNODEX
     +           CNTROL(3),IOUTER,IPHASE,NTIMES,IDLIFE)                UNODEX
D        WRITE(6,995)                                                   UNODEX
  995   FORMAT(/,1X,'RETURNED FROM MODULE ERPROP')                      UNODEX
   50   CONTINUE                                                        UNODEX
                                                                        UNODEX
C.. SORT AND PRINT OUTPUT                                               UNODEX
                                                                        UNODEX
      CALL RSORT(DS,IVIR,NVIR,UT,LT)                                    UNODEX
        DO 3029 I=1,NVIR                                                UNODEX
        J=IVIR(I)                                                       UNODEX
        DSM=-DS(I)                                                      UNODEX
        WRITE(2,2020)IVIR(I),LVIR(1,J),LVIR(2,J),DSM,DDS(J)             UNODEX
 2020   FORMAT(1X,I5,'-',2I3,1P2E15.6)                                  UNODEX
 3029   CONTINUE                                                        UNODEX
                                                                        UNODEX
                                                                        UNODEX
C***********************************************************************UNODEX
C*                  BEGINNING ECHELON EVALUATION                       *UNODEX
C***********************************************************************UNODEX
                                                                        UNODEX
        IPHASE=3                                                        UNODEX
```

```
      DO 1010 IOUTER=1,NVIR                                              UNODEX
      CNTROL(3)=NLAB+IOUTER                                              UNODEX
      INT3=CNTROL(3)                                                     UNODEX
      WRITE(6,1100) IOUTER                                               UNODEX
 1100 FORMAT(//,1X,'PHASE 3 *** ADDING EXPERIMENT NUMBER: ',I4)          UNODEX
                                                                         UNODEX
     CALL ADVIRT(IOUTER,NLAB,X(1,INT3),Y(1,INT3),E(1,INT3),              UNODEX
    +            PARAM,NPARAM,INT3)                                      UNODEX
                                                                         UNODEX
D     WRITE(6,1101)                                                      UNODEX
 1101 FORMAT(1X,'BACK FROM ADVIRT')                                      UNODEX
                                                                         UNODEX
     CALL FITSALL(INT3,PARAM,NPARAM,AC,SUMC,IBCHN,NTLNS)                 UNODEX
                                                                         UNODEX
D     WRITE(6,1102)                                                      UNODEX
 1102 FORMAT(1X'BACK FROM FITSALL')                                      UNODEX
                                                                         UNODEX
     CALL ERPROP(PARAM,NPARAM,AC,SUMC,NB,NIV,CNTROL(19),                 UNODEX
    +            CNTROI(3),IOUTER,IPHASE,NTIMES,IDLIFE)                  UNODEX
                                                                         UNODEX
D     WRITE(6,1103)                                                      UNODEX
 1103 FORMAT(1X'BACK FROM ERPROP')                                       UNODEX
 1010 CONTINUE                                                           UNODEX
                                                                         UNODEX
C.. WRITE PLOTTER INFO TO UNIT 3                                         UNODEX
                                                                         UNODEX
                                                                         UNODEX
      WRITE(6,1115)                                                      UNODEX
 1115 FORMAT(//,                                                         UNODEX
    +       '   VIRTUAL        DELTA         FRACTIONAL',/,            UNODEX
    +       '    DATA        UNCERTAINTY    UNCERTAINTY',/,            UNODEX
    +       '   NUMBER        REDUCTION      REDUCTION')                UNODEX
      DO 3030 I=1,NVIR                                                   UNODEX
      J=IVIR(I)                                                          UNODEX
      DSM=-DS(I)                                                         UNODEX
                                                                         UNODEX
      WRITE(2,2020) IVIR(I),LVIR(1,J),LVIR(2,J),DSM,DDS(J)               UNODEX
      WRITE(6,2020) IVIR(I),LVIR(1,J),LVIR(2,J),DSM,DDS(J)               UNODEX
3030  CONTINUE                                                           UNODEX
                                                                         UNODEX
      JADD=0                                                             UNODEX
      IF(NVIR.LT.3)GOTO 4200                                             UNODEX
      DELO=-DS(1)                                                        UNODEX
      DEL1=DELO                                                          UNODEX
      DEL2=1.0E-10                                                       UNODEX
                                                                         UNODEX
      DO 4100 I=2,NVIR                                                   UNODEX
      DEL=DS(I-1)-DS(I)                                                  UNODEX
      JADD=I-1                                                           UNODEX
      IF(ABS(DEL/DELO).LT.ADEL)GOTO 4200                                 UNODEX
      DEL3=DEL2                                                          UNODEX
      DEL2=DEL1                                                          UNODEX
      DEL1=DEL                                                           UNODEX
      IF(I.GT.3)DELO=(DEL1+DEL2+DEL3)/3                                  UNODEX
      IF(I.EQ.2)DELO=(DEL1+DEL2)/2                                       UNODEX
4100  CONTINUE                                                           UNODEX
4200  CONTINUE                                                           UNODEX
      DO 4500 I=1,JADD                                                   UNODEX
```

```
        J=IVIR(I)                                                       UNODEX
 4500   WRITE(8,4510) IVIR(I),LVIR(1,J),LVIR(2,J),-DS(I),DDS(J),       UNODEX
     +                SIGREF(IDLIFE),SIGREF(IDLIFE)+DS(I)              UNODEX
 4510   FORMAT(1X,I5,'-',2I3,1P4E15.6)                                  UNODEX
        IF(JADD.GT.0.AND.JADD.LT.NVIR) GOTO 2222                        UNODEX
                                                                        UNODEX
C.. HERE A CALL TO PLOTTING ROUTINES MAY BE PROVIDED                    UNODEX
                                                                        UNODEX
        STOP                                                            UNODEX
        END                                                             UNODEX
      SUBROUTINE GENVIRT(NAME,NIV,XH,XL,NLEV,NVIR)                      GENVIR
                                                                        GENVIR
       PARAMETER NVMAX=1250                                             GENVIR
       CHARACTER*12 NAME                                                GENVIR
       DIMENSION X(6,10)                    !INDEPENDENT VARIABLES      GENVIR
       DIMENSION I(6)                                                   GENVIR
       DIMENSION NAME(1), XH(1), XL(1), NLEV(1)                         GENVIR
       COMMON/XV/XVIR(5,NVMAX),IVIR(NVMAX),LVIR(2,NVMAX),               GENVIR
     +             DS(NVMAX),DDS(NVMAX),YVIR(NVMAX)                   GENVIR
                                                                        GENVIR
D      WRITE(6,990)                                                     GENVIR
D  990  FORMAT(/,1X,'ENTERED GENVIRT.FOR')                              GENVIR
                                                                        GENVIR
C.. CALCULATE NLEV(K) EQUAL SPACED LEVELS FOR EACH OF THE K             GENVIR
C   INDEPENDENT VARIABLES SO THAT THE HIGH XH(K), AND LOW, XL(K)        GENVIR
C   ARE THE ENDPOINTS                                                   GENVIR
                                                                        GENVIR
       LIMIT=10                                                         GENVIR
                                                                        GENVIR
       NUMRECS=1                                                        GENVIR
       DO 30 K=1,NIV                                                    GENVIR
D      WRITE(6,*)'GENVIRT DO 30: K=',K                                  GENVIR
                                                                        GENVIR
       NLEVK=NLEV(K)                                                    GENVIR
       DO 27 J=1,NLEVK                                                  GENVIR
D      WRITE(6,*)'GENVIRT DO 27: J=',J                                  GENVIR
       JJ=J-1                                                           GENVIR
       DELX=(XH(K)-XL(K))/FLOAT(NLEVK-1)                                GENVIR
       X(K,J)=XL(K)+FLOAT(JJ)*DELX                                      GENVIR
   27  CONTINUE                                                         GENVIR
       NUMRECS=NUMRECS*NLEV(K)                                          GENVIR
   30  CONTINUE                                                         GENVIR
                                                                        GENVIR
       DO 40 INIVS=1,NIV                                                GENVIR
       NLEVI=NLEV(INIVS)                                                GENVIR
       WRITE(6,130)NAME(INIVS),(X(INIVS,INLEV),INLEV=1,NLEVI)           GENVIR
  130  FORMAT(/,1X,A12,5(1X,F10.4))                                     GENVIR
   40  CONTINUE                                                         GENVIR
                                                                        GENVIR
       WRITE(3,185)NUMRECS                                              GENVIR
  185  FORMAT(I5)                                                       GENVIR
                                                                        GENVIR
       INOREC=1                                                         GENVIR
                                                                        GENVIR
       WRITE(6,*)' NIV = ',NIV                                          GENVIR
                                                                        GENVIR
       NLEV1=NLEV(1)                                                    GENVIR
       NLEV2=NLEV(2)                                                    GENVIR
```

```
      NLEV3=NLEV(3)                                                    GENVIR
      NLEV4=NLEV(4)                                                    GENVIR
      NLEV5=NLEV(5)                                                    GENVIR
      NLEV6=NLEV(6)                                                    GENVIR
      IF(NIV.LT.6)NLEV6=0                                              GENVIR
      IF(NIV.LT.5)NLEV5=0                                              GENVIR
      IF(NIV.LT.4)NLEV4=0                                              GENVIR
      IF(NIV.LT.3)NLEV3=0                                              GENVIR
      IF(NIV.LT.2)NLEV2=0                                              GENVIR
                                                                       GENVIR
      GOTO (1,2,3,4,5,6),NIV                                           GENVIR
                                                                       GENVIR
    6 I6=0                                                             GENVIR
   66 I6=I6+1                                                          GENVIR
    5 I5=0                                                             GENVIR
   55 I5=I5+1                                                          GENVIR
    4 I4=0                                                             GENVIR
   44 I4=I4+1                                                          GENVIR
    3 I3=0                                                             GENVIR
   33 I3=I3+1                                                          GENVIR
    2 I2=0                                                             GENVIR
   22 I2=I2+1                                                          GENVIR
    1 I1=0                                                             GENVIR
   11 I1=I1+1                                                          GENVIR
      I(6)=I6                                                          GENVIR
      I(5)=I5                                                          GENVIR
      I(4)=I4                                                          GENVIR
      I(3)=I3                                                          GENVIR
      I(2)=I2                                                          GENVIR
      I(1)=I1                                                          GENVIR
      DO 42 M=1,NIV                                                    GENVIR
      IM=I(M)                                                          GENVIR
   42 X(M,LIMIT)=X(M,IM)                                               GENVIR
      WRITE(3,175)INOREC,(I(M),M=1,NIV),(X(M,LIMIT),M=1,NIV)           GENVIR
  175 FORMAT(1X,'V',I4,'X',5I1,1P5E11.4)                               GENVIR
      WRITE(6,180)INOREC,(I(M),M=1,NIV)                                GENVIR
  180 FORMAT(1X,'V',I4,'X',5I1)                                        GENVIR
      DO 832 M=1,NIV                                                   GENVIR
      XVIR(M,INOREC)=X(M,LIMIT)                                        GENVIR
  832 CONTINUE                                                         GENVIR
      IVIR(INOREC)=INOREC                                              GENVIR
      LVIR(1,INOREC)=I1*10+I2                                          GENVIR
      LVIR(2,INOREC)=I3*100+I4*10+I5                                   GENVIR
      INOREC=INOREC+1                                                  GENVIR
      IF(I1.LT.NLEV1)GOTO 11                                           GENVIR
      IF(I2.LT.NLEV2)GOTO 22                                           GENVIR
      IF(I3.LT.NLEV3)GOTO 33                                           GENVIR
      IF(I4.LT.NLEV4)GOTO 44                                           GENVIR
      IF(I5.LT.NLEV5)GOTO 55                                           GENVIR
      IF(I6.LT.NLEV6)GOTO 66                                           GENVIR
      NVIR=INOREC-1                                                    GENVIR
      RETURN                                                           GENVIR
      END                                                              GENVIR
     SUBROUTINE BWRITE(NLAB)                                           BWRITE
C ********************************************************************* BWRITE
C *      THE BWRITE ROUTINE READS THE MODEL BUILDING CORROSION DATA   * BWRITE
C *      FROM FILE MBCOR1.DAT ON CHANNEL 1 INTO COMMON ARRAYS X AND Y.* BWRITE
C *                                                                   * BWRITE
```

```
C *      NLAB=       NUMBER OF LABORATORY-MEASURED MODEL BUILDING DATA  * BWRITE
C *      NVIR=       NUMBER OF VIRTUAL IV DATA CONTAINED IN VIRCOR.DAT  * BWRITE
C *      Y(1,M)      OBSERVED VALUE OF CORROSION RATE (THE ONLY DV)     * BWRITE
C *                     FOR THE M-TH DATA                               * BWRITE
C *      X(I,M)      MEASURED VALUE OF THE I-TH I.V. FOR THE M-TH DATA  * BWRITE
C *                                                                     * BWRITE
C *      DURING DEVELOPMENT THE BWRITE ROUTINE READ THE MODEL BUILDING * BWRITE
C *       DATA AND WROTE IT TO A BINARY STORAGE FILE, HENCE THE SOME    * BWRITE
C *       WHAT UNFITTINE NAME - B(inary)WRITE.FOR                       * BWRITE
C ********************************************************************* BWRITE
         PARAMETER NDTS=1250                                            BWRITE
         COMMON X(6,NDTS),Y(1,NDTS),E(1,NDTS)                           BWRITE
         COMMON/BB/LAB(7,500)                                           BWRITE
                                                                        BWRITE
D        WRITE(6,990)                                                   BWRITE
  990    FORMAT(/,1X,'ENTERED MODULE BWRITE')                           BWRITE
                                                                        BWRITE
         READ(1,490) NLAB                                               BWRITE
  490    FORMAT(I4)                                                     BWRITE
         DO 20 IBWRT1=1,NLAB                                            BWRITE
         READ(1,505) (LAB(K,IBWRT1),K=1,4),Y(1,IBWRT1),(X(J,IBWRT1),   BWRITE
     +              J=1,4),X(6,IBWRT1),X(5,IBWRT1),(LAB(K,IBWRT1),K=5,7)BWRITE
  504    FORMAT(1X,2A2,1X,A1,1X,A2,1X,F8.3,1X,F4.0,1X,F5.2,1X,F7.5,     BWRITE
     + 1X,F3.0,1X,F5.0,1X,F6.0,2X,3A2)                                  BWRITE
   20    CONTINUE                                                       BWRITE
         CLOSE(UNIT=1)                                                  BWRITE
         WRITE(6,991)NLAB                                               BWRITE
  991    FORMAT(I4,'  MODEL BUILDING DATA RECORDS READ')                BWRITE
  505    FORMAT(2A2,1X,A1,1X,A2,1X,F5.2,26X,F3.0,1X,F4.2,1X,F6.5,       BWRITE
     +          1X,F2.0,1X,F4.0,1X,F5.0,2X,3A2)                         BWRITE
         RETURN                                                         BWRITE
         END                                                            BWRITE
       SUBROUTINE ADVIRT(IOUTER,NM1,X,Y,E,PARAM,NPARAM,NIV)             ADVIRT
C ********************************************************************* ADVIRT
C    THE ADVIRT ROUTINE EVALUATES THE DV FROM THE VIRTUAL IV DATA       ADVIRT
C    AND ADDS THE VIRTUAL DATA TO THE MODEL BUILDING DATABASE FILE      ADVIRT
C    MBCOR.DAT                                                          ADVIRT
C                                                                       ADVIRT
C       Y(1) = CORROSION RATE (DV)                                      ADVIRT
C                                                                       ADVIRT
C       X(1)=TEMP                                                       ADVIRT
C       X(2)=OX                                                         ADVIRT
C       X(3)=MG                                                         ADVIRT
C       X(4)=H2O                                                        ADVIRT
C       X(5)=TOT TIME                                                   ADVIRT
C ********************************************************************* ADVIRT
         PARAMETER NVMAX=1250                                           ADVIRT
         DIMENSION X(1),Y(1),PARAM(1),E(1)                              ADVIRT
         COMMON/CORDAT/XX(6)                                            ADVIRT
         COMMON/LABEL/LLAB(2)                                           ADVIRT
         COMMON/XV/XVIR(5,NVMAX),IVIR(NVMAX),LVIR(2,NVMAX),             ADVIRT
     +             DS(NVMAX),DDS(NVMAX),YVIR(NVMAX)                     ADVIRT
                                                                        ADVIRT
D        WRITE(6,990)                                                   ADVIRT
  990    FORMAT(/,1X,'ENTERED MODULE ADVIRT')                           ADVIRT
                                                                        ADVIRT
         JJ=IVIR(IOUTER)                                                ADVIRT
         DO 40 J=1,5                                                    ADVIRT
```

```
   40     XX(J)=XVIR(J,JJ)                                                ADVIRT
                                                                          ADVIRT
          WRITE(6,508)IVIR(IOUTER),LVIR(1,JJ),LVIR(2,JJ)                  ADVIRT
          WRITE(2,508)IVIR(IOUTER),LVIR(1,JJ),LVIR(2,JJ)                  ADVIRT
  508     FORMAT(/,'  ADDED VIRTUAL DATA POINT    ',                      ADVIRT
     +           '[ V',I5,'-',2I3,']')                                    ADVIRT
                                                                          ADVIRT
C..  EVALUATE THE DV (Y) FROM THE IV'S                                    ADVIRT
                                                                          ADVIRT
          WRITE(6,*) 'XX=',(XX(I),I=1,6)                                  ADVIRT
          DO 1 I=1,6                                                      ADVIRT
    1     X(I)=XX(I)                                                      ADVIRT
          Y(1)=YO(X,NIV,PARAM,NPARAM,IDV)                                 ADVIRT
          YVIR(JJ)=Y(1)                                                   ADVIRT
          E(1)=ERE(X)                                                     ADVIRT
                                                                          ADVIRT
          WRITE(2,*)'Y,E=',Y(1),E(1)                                      ADVIRT
          WRITE(6,*)'Y,E=',Y(1),E(1)                                      ADVIRT
                                                                          ADVIRT
          RETURN                                                          ADVIRT
          END                                                             ADVIRT
       FUNCTION ERE(X)                                                    ERE
C ************************************************************************ ERE
C     ERE EVALUATES AN EMPIRICALLY-CONSISTENT ERROR,                      ERE
C     IN IV UNITS, FOR THE VIRTUAL DATA IN THE EXPERIMENT SAMPLE          ERE
C     SPACE.                                                              ERE
C                                                                         ERE
C     THE EXAMPLE BELOW WAS DETERMINED BY LINEAR REGRESSION ON            ERE
C     THE DATA IN THE MODEL BUILDING DATABASE.                            ERE
C                                                                         ERE
C     EXAMPLE:                                                            ERE
C                                                                         ERE
C     ERE=C(1)*X(1)+C(2)*X(2)+C(3)*X(3)+C(4)*X(4)+C(5)/SQRT(X(5))         ERE
C                                                                         ERE
C     COMMENT:                                                            ERE
C     NOTE THE FOLLOWING FORM OF THE 'VIRTUAL' DATA ERROR                 ERE
C                                                                         ERE
C ************************************************************************ ERE
          DIMENSION X(1)                                                  ERE
                                                                          ERE
          ERE=     1.27402 *X(1)                                          ERE
     +            -14.7625 *X(2)                                         ERE
     +            +595.031 *X(3)                                         ERE
     +            -0.143878*X(4)                                         ERE
     +            +173.812/SQRT(X(5))                                    ERE
                                                                          ERE
C1.26714*X(1)-21.3949*X(2)+692.679*X(3)-0.215448*X(4)                     ERE
C     +         +248.000/SQRT(X(5))                                       ERE
                                                                          ERE
          RETURN                                                          ERE
          END                                                             ERE
       SUBROUTINE FITSALL(INT3,PARAM,NPARAM,AC,SUMC,IBCHN,NTLNS)          FITSAL
C ************************************************************************ FITSAL
C    THE FITSALL MODULE IS THE DRIVER FOR DETERMINING THE MAXIMUM         FITSAL
C    LIKLEIHOOD ESTIMATES OF THE NONLINEAR-MULTIVARIABLE PARAMETERS       FITSAL
C                                                                         FITSAL
C    IT SETS UP THE REGRESSION CONTROLS AND CONVERGENVCE CRITERIA AND     FITSAL
C    CONTROLS THE CALLING SEQUENCE TO THE VARIOUS SPECIALIZED MODULES     FITSAL
```

```
C     SUCH AS GAUSSIAN REDUCTION, MATRIX INVERSION, CONVERGENCE TESTS    FITSAL
C     WORKING ARRAY MANIPULATION AND UPDATING, ETC.                      FITSAL
C                                                                        FITSAL
C ********************************************************************** FITSAL
          DIMENSION BTRIAL(20),PARAM(NPARAM),CORE(12500)                 FITSAL
          INTEGER CNTROL,BDIM                                            FITSAL
          CHARACTER*80 TITLE                                             FITSAL
          COMMON/TITLE/TITLE(5)                                          FITSAL
          COMMON/CNTROL/CNTROL(25)                                       FITSAL
          COMMON/CONVG/SCONVG,PCONVG,BCONVG                              FITSAL
          CHARACTER*4 NPRINT(5),IPRINT(2)                                FITSAL
          CHARACTER*9 IFORM(8)                                           FITSAL
          DIMENSION AC(1),IDAT(3),ITYM(3)                                FITSAL
          CHARACTER*8 TOD                                                FITSAL
          CHARACTER*9 MDY                                                FITSAL
                                                                         FITSAL
          DATA IFORM/'  1.0               ',                             FITSAL
         +' 1/OBS              ',                                        FITSAL
         +'1/CALC              ',                                        FITSAL
         +'  OBS               ',                                        FITSAL
         +'  CALC              ',                                        FITSAL
         +'1/Z(C5,N)           ',                                        FITSAL
         +' Z(C5,N)            ',                                        FITSAL
         +'1/MX(0,C)           '/                                        FITSAL
          DATA IPRINT/' NO ','YES '/                                     FITSAL
                                                                         FITSAL
          BIN(K,J)= 0.5- 0.5 *(-1.) ** (K/2 **(J-1))                     FITSAL
                                                                         FITSAL
D         WRITE(6,990)                                                   FITSAL
  990     FORMAT(/,1X,'ENTERED MODULE FITSALL')                          FITSAL
                                                                         FITSAL
C.. DEFAULT CONVERGENCE CRITERIA (IF NOT SET ON INPUT)                   FITSAL
          IF(BCONVG.LE.0..AND.PCONVG.LE.0.)BCONVG=1.E-2                  FITSAL
          IF(PCONVG.LE.0.)PCONVG=1.E-5                                   FITSAL
          IF(SCONVG.LE.0.)SCONVG=1.E-12                                  FITSAL
                                                                         FITSAL
          CNTROL(3)=-INT3                  ! # DATA POINTS (ABS VAL)     FITSAL
                                                                         FITSAL
C.. NOTE: FOLLOWING INPUT CONTROLS MAY BE CHANGED DURING PROCESSING:     FITSAL
C     CNTROL(1), WILL BE READ FROM CHAN 12, AND MAY BE CHANGED BY YCOMP  FITSAL
C     CNTROL(2), WILL BE READ FROM CHANNEL 12                            FITSAL
C     CNTROL(10), MAY BE ALTERED BY GAUSS.FR                             FITSAL
C     CNTROL(11), MAY BE RESET TO 0 BY GAUSS.FOR                         FITSAL
C     CNTROL(12), MAY BE RESET TO 0 BY GAUSS.FOR                         FITSAL
                                                                         FITSAL
          KNTR8 =CNTROL(8)                                               FITSAL
          KNTR10=CNTROL(10)    ! PARAMETER VARIATIONS                    FITSAL
          KNTR11=CNTROL(11)                                              FITSAL
          KNTR12=CNTROL(12)                                              FITSAL
          KNTR19=CNTROL(19)                                              FITSAL
          MDIM=CNTROL(5)       ! # VARIABLES                             FITSAL
          IF (CNTROL(8).EQ.6.OR.CNTROL(8).EQ.7) MDIM=MDIM+1              FITSAL
          NDIM=IABS(CNTROL(3))! # DATA POINTS                            FITSAL
          IF(CNTROL(16).LE.0)CNTROL(16)=1                                FITSAL
          III=CNTROL(16)                                                 FITSAL
                                                                         FITSAL
C.. OUTER LOOP OVER III PROBLEMS                                         FITSAL
                                                                         FITSAL
```

```
      DO 1000 II=1,III                                                  FITSAL
                                                                        FITSAL
C      WRITE(6,991)II                                                   FITSAL
  991 FORMAT(/,3X,'DO 1000: II=',I3)                                    FITSAL
                                                                        FITSAL
      CNTROL(23)=II                                                     FITSAL
      IF(CNTROL(16).LE.1)GOTO 35                                        FITSAL
                                                                        FITSAL
C.. AT THIS POINT, STATEMENTS MAY BE ENTERED FOR INPUTTING INFORMATION  FITSAL
C     ABOUT II-TH PROBLEM SUCH AS CONTROL(3), CNTROL(5), CNTROL(17),    FITSAL
C     CNTROL(18), ETC.                                                  FITSAL
C                                                                       FITSAL
C                                                                       FITSAL
C                                                                       FITSAL
C                                                                       FITSAL
                                                                        FITSAL
                                                                        FITSAL
   35 LAST=1                                                            FITSAL
      IF(CNTROL(17).LE.0)CNTROL(17)=1                                   FITSAL
      IF(CNTROL(18).LE.0)CNTROL(18)=1                                   FITSAL
      BB=0.4*ALOG10(PCONVG)                                             FITSAL
      IF(BCONVG.LE.0.)BCONVG=10.**BB                                    FITSAL
      NSETS=CNTROL(17)                                                  FITSAL
                                                                        FITSAL
C.. READ IN NSETS OF GUESSES                                            FITSAL
      DO 50 L=1,NSETS                                                   FITSAL
C      WRITE(6,992)L                                                    FITSAL
  992 FORMAT(/,5X,'DO 50: L=',I3)                                       FITSAL
      READ(IBCHN,40)IB,IC,(BTRIAL(I),I=1,IB)                            FITSAL
   40 FORMAT(2I5,7E11.4,(/,8E11.4))                                     FITSAL
C      WRITE(2,44)L,IB,IC,(BTRIAL(I),I=1,IB)                           FITSAL
C   44  FORMAT(3I5,1P7E15.5/(15X,7E15.5))                               FITSAL
      I=0                                                               FITSAL
      LASTP2=LAST+2                                                     FITSAL
      NEXT=LASTP2+IB-1                                                  FITSAL
                                                                        FITSAL
      DO 45 K=LASTP2,NEXT                                               FITSAL
                                                                        FITSAL
      I=I+1                                                             FITSAL
   45 CORE(K)=BTRIAL(I)                                                 FITSAL
      CORE(LAST)=IB                                                     FITSAL
      LASTP1=LAST+1                                                     FITSAL
      CORE(LASTP1)=IC                                                   FITSAL
   50 LAST=NEXT+1                                                       FITSAL
                                                                        FITSAL
C....SET UP MEMORY LOCATIONS IN CORE-ARRAY                              FITSAL
      BDIM=CNTROL(4)                                                    FITSAL
      LOCZ=4*BDIM+LAST                                                  FITSAL
      LOCA=LOCZ+MDIM*NDIM+1                                             FITSAL
      MINDIM=LOCA+BDIM*BDIM-1                                           FITSAL
      WRITE(6,333) MINDIM                                               FITSAL
      WRITE(2,333) MINDIM                                               FITSAL
  333 FORMAT(/,1X'MINIMUM CORE DIMENSION ='I8)                          FITSAL
      NEXT=1                                                            FITSAL
C....THE FOLLOWING ERRORH VALUE HAS BEEN CHANGED -  1.E60 TO 1.0E38     FITSAL
      ERRORH=1.0E38                                                     FITSAL
                                                                        FITSAL
C.. LOOP OVER NSETS SETS OF GUESSES                                     FITSAL
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```
      DO 200 K=1,NSETS                                                  FITSAL
C      WRITE(6,993)K                                                    FITSAL
  993 FORMAT(/,7X,'DO 200: K=',I3)                                      FITSAL
      CNTROL(24)=K                                                      FITSAL
                                                                        FITSAL
C.. RESET CNTROL(10-12) IN CASE THEY WERE ALTERED ON PREVIOUS PASS      FITSAL
      CNTROL(10)=KNTR10                                                 FITSAL
      CNTROL(11)=KNTR11                                                 FITSAL
      CNTROL(12)=KNTR12                                                 FITSAL
                                                                        FITSAL
C.. SET CNTROL(1-2) FOR THIS SET OF GUESSES                             FITSAL
      CNTROL(2)=CORE(NEXT)    ! IB=TOTAL # PARS FOR THIS TRIAL SET      FITSAL
      CNTROL(1)=CORE(NEXT+1) ! IC=#PARAMS TO BE FITTED FOR TRIAL SET    FITSAL
      M3=CNTROL(2)                                                      FITSAL
                                                                        FITSAL
C.. STARTING LOCATION FOR B-ARRAY FOR THIS SET OF GUESSES               FITSAL
      LOCB=LAST                                                         FITSAL
                                                                        FITSAL
C.. INITIALIZE PARAMETER VALUES AT GUESSES                              FITSAL
      DO 80 I=1,M3                                                      FITSAL
      LASTP1=LAST+I-1                                                   FITSAL
   80 CORE(LASTP1)=CORE(NEXT+1+I)                                       FITSAL
                                                                        FITSAL
C.. UP-DATE "NEXT" TO BE READY TO DO THE NEXT PASS THRU THE DO 200 LOOP FITSAL
      NEXT=NEXT+M3+2                                                    FITSAL
                                                                        FITSAL
C.. SET PARAMETERS FOR THIS PASS                                        FITSAL
      NB=CNTROL(1)                  ! # PARAMETERS BEING FITTED       FITSAL
      NPTS=IABS(CNTROL(3))          ! # DATA POINTS                   FITSAL
      NVARS=CNTROL(5)               ! TOTAL # VARIABLES               FITSAL
      LIMIT=CNTROL(6)               ! LIMIT ON # ITERATIONS           FITSAL
                                                                        FITSAL
C.. DOCUMENT SETTINGS                                                   FITSAL
      WRITE(2,4)                                                        FITSAL
    4 FORMAT(1X,'NONLINEAR REGRESSION CONTROLS ARE:')                   FITSAL
      WRITE (2,53) (MRULER,MRULER=1,19)                                 FITSAL
   53 FORMAT(6X,19I5)                                                   FITSAL
      WRITE (2,55) (CNTROL(I),I=1,19)                                   FITSAL
   55 FORMAT(6X,19I5)                                                   FITSAL
      WRITE(2,25)NB,NPTS,NVARS,LIMIT                                    FITSAL
   25 FORMAT(                                                           FITSAL
     + 1X,'NUMBER OF PARAMETERS                ',I12,/,                 FITSAL
     + 1X,'NUMBER OF DATA POINTS               ',I12,/,                 FITSAL
     + 1X,'NUMBER OF VARIABLES                 ',I12,/,                 FITSAL
     + 1X,'LIMIT ON NUMBER OF ITERATIONS       ',I12,/)                 FITSAL
                                                                        FITSAL
C.. CHANGED WORDING OF FOLLOWING STATEMENT *********                    FITSAL
C.. DOCUMENT CONVERGENCE CRITERIA                                       FITSAL
      WRITE(2,111)SCONVG,PCONVG,BCONVG                                  FITSAL
  111 FORMAT(' CONVERGENCE CRITERIA:',                                  FITSAL
     +       6X,'SCONVG =',1PE11.3,                                     FITSAL
     +       6X,'PCONVG =',E11.3,                                       FITSAL
     +       6X,'BCONVG =',E11.3)                                       FITSAL
                                                                        FITSAL
C.. IS INTERMEDIATE OUTPUT WANTED ?                                     FITSAL
      IF(CNTROL(7).NE.0)GOTO 18                                         FITSAL
      WRITE(2,11)                                                       FITSAL
   11 FORMAT(' CNTROL(7) = 0, SO NO INTERMEDIATE OUTPUT')               FITSAL
```

```
      GOTO 19                                                          FITSAL
   18 WRITE(2,9)                                                       FITSAL
    9 FORMAT (/,1X,'THE FOLLOWING INFORMATION IS TO BE PRINTED OUT:'/FITSAL
     +' INPUT DATA   SUMSQ AND PARAMETER VALUES   NORMAL EQ MATRICES', FITSAL
     +'  RESTRAINED CHANGE MECHANISM    POINT BY POINT COMPARISON')    FITSAL
                                                                       FITSAL
C....IDENTIFY INTERMEDIATE PRINT OPTIONS SELECTED                      FITSAL
      DO 22 J=1,5                                                      FITSAL
      L=1                                                              FITSAL
      IF(BIN(CNTROL(7),J).GT.0.)L=2                                    FITSAL
      NPRINT(J)=IPRINT(L)                                              FITSAL
   22 CONTINUE                                                         FITSAL
                                                                       FITSAL
      WRITE(2,21)(NPRINT(J),J=1,5)                                     FITSAL
   21 FORMAT (5X,A3,18X,A3,21X,A3,25X,A3,28X,A3,/)                     FITSAL
                                                                       FITSAL
C.. SET AND DOCUMENT LL=WEIGHTING FCN INDEX                            FITSAL
   19 LL=CNTROL(8)                                                     FITSAL
      WRITE(2,12)CNTROL(8),IFORM(LL)                                   FITSAL
   12 FORMAT(' CNTROL(8) =',I3,' SO MINIMIZE LEAST SQUARES             FITSAL
     +       WEIGHTED BY (',A9,' )')                                   FITSAL
                                                                       FITSAL
C...DOCUMENT RESTRAINED CHANGE MECHANISM                               FITSAL
      IF(CNTROL(10).EQ.0)WRITE(2,15)                                   FITSAL
   15 FORMAT(' CNTROL(10) = 0, SO UNCONSTRAINED PARAMETER CHANGES')    FITSAL
                                                                       FITSAL
C.. NOTE: POSITIVE CNTROL(10) IS IN UNITS OF TENS OF PERCENT           FITSAL
      ICHANG=CNTROL(10)*10                                             FITSAL
      IF(CNTROL(10).NE.0)WRITE(2,14)ICHANG                             FITSAL
   14 FORMAT(' CNTROL(10) NONZERO, PARAMETERS CAN CHANGE BY AT MOST',FITSAL
     +       I4,' PERCENT')                                            FITSAL
                                                                       FITSAL
C.. DOCUMENT STARTING GUESSES FOR THIS PASS                            FITSAL
      WRITE(2,7)                                                       FITSAL
    7 FORMAT(1X,'STARTING GUESSES FOR THE PARAMETERS B(J)')            FITSAL
      LASPM3=LAST+M3-1                                                 FITSAL
      WRITE (2,60) (JPC,JPC=1,M3)                                      FITSAL
   60 FORMAT(6X,'  J :',6X,I2,8(11X,I2))                              FITSAL
      WRITE(2,3)(CORE(I),I=LAST,LASPM3)                                FITSAL
    3 FORMAT(6X,'B(J):'1P10E13.4)                                      FITSAL
                                                                       FITSAL
C.. DOCUMENT ARRAY DIMENSIONS                                          FITSAL
      WRITE(2,8)MD,M,NDIM,BDIM                                         FITSAL
    8 FORMAT(/,1X,'NONLINEAR REGRESSION ARRAY DIMENSIONS ARE:',/,      FITSAL
     +       6X,'ERROR MATRIX:        Z(',I2,',',I3,')',/,           FITSAL
     +       6X,'PARAMETERS:          B(',I2,')',/)                  FITSAL
                                                                       FITSAL
      IF(BIN(CNTROL(7),2).GT.0.)WRITE(2,70)                            FITSAL
   70 FORMAT(///,'*********************************************',/,FITSAL
     +          '* BEGIN INTERMEDIATE NORMAL EQUATION MATRICIES*',/,FITSAL
     +          '*********************************************',/)FITSAL
                                                                       FITSAL
                                                                       FITSAL
                                                                       FITSAL
                                                                       FITSAL
C.. SET INITIAL ENTRY FLAG FOR YCOMP.FR AND GAUSS.FR                   FITSAL
      CNTROL(22)=1                                                     FITSAL
                                                                       FITSAL
```

```
C.. CNTROL(3) < 0  ON 1ST PASS OF  ?                                    FITSAL
C.. K=1  ON 1ST PASS OF DO 200 LOOP                                     FITSAL
C.. FILL CORE(  )  FROM  LOCZ  TO  LOCZ+NDIM*MDIM-1  WITH OBSERVED DATA FITSAL
      IF(CNTROL(3).LT.0.AND.K.EQ.1)Y=YCOMP(1,CORE(LAST),CORE(LOCZ),     FITSAL
     +     MDIM,NDIM,BDIM)                                            FITSAL
      IF(NPTS.NE.IABS(CNTROL(3)))NPTS=IABS(CNTROL(3))                   FITSAL
      IF(BIN(CNTROL(7),1).EQ.1.)CALL PRINDA(CNTROL,CORE(LOCZ),MDIM,     FITSAL
     +                                      NDIM)                     FITSAL
                                                                        FITSAL
C.. PERFORM FITTING TO MINIMIZE ERROR                                   FITSAL
      CALL GAUSS(CORE(LOCB),CORE(LOCZ),MDIM,NDIM,BDIM CORE(LOCA))       FITSAL
                                                                        FITSAL
C.. COMPUTE ERRORS & UNCERTAINTIES, AND OUTPUT RESULTS                  FITSAL
      CALL FINALE(CORE(LOCB),CORE(LOCZ),MDIM,NDIM,BDIM,CORE(LOCA),      FITSAL
     +            ERROR,SUMSQ)                                        FITSAL
                                                                        FITSAL
      IF(CNTROL(21).EQ.0)WRITE(6,107)                                   FITSAL
      IF(CNTROL(21).EQ.1)WRITE(6,102)PCONVG                             FITSAL
      IF(CNTROL(21).EQ.2)WRITE(6,103)SCONVG                             FITSAL
      IF(CNTROL(21).EQ.3)WRITE(6,104)                                   FITSAL
      IF(CNTROL(21).EQ.4)WRITE(6,105)                                   FITSAL
      IF(CNTROL(21).EQ.5)WRITE(6,106)                                   FITSAL
      IF(CNTROL(21).EQ.0)WRITE(2,107)                                   FITSAL
      IF(CNTROL(21).EQ.1)WRITE(2,102)PCONVG                             FITSAL
      IF(CNTROL(21).EQ.2)WRITE(2,103)SCONVG                             FITSAL
      IF(CNTROL(21).EQ.3)WRITE(2,104)                                   FITSAL
      IF(CNTROL(21).EQ.4)WRITE(2,105)                                   FITSAL
      IF(CNTROL(21).EQ.5)WRITE(2,106)                                   FITSAL
102   FORMAT (//,1X,'CAUCHY CONVERGENCE OF PARAMETER ISS.'              FITSAL
     +        '  NO PARAMETER ESTIMATED TO NEED FRACTIONAL CHANGE       FITSAL
     +        EXCEEDING',1PE11.3)                                     FITSAL
103   FORMAT (//,1X,'CAUCHY CONVERGENCE OF SUM OF SQUARES.',            FITSAL
     +        '  FRACTIONAL REDUCTION IN MINIMUM SUMSQ IS LESS THAN',  FITSAL
     +        1PE11.3)                                                FITSAL
104   FORMAT (//,1X,'TERMINATION DUE TO LIMIT ON NUMBER OF ',           FITSAL
     +        'ITERATIONS')                                           FITSAL
105   FORMAT (//,1X,'TERMINATION DUE TO SINGULARITY OF NORMAL EQS ')    FITSAL
106   FORMAT (//,1X,'NO SUM OF SQUARES REDUCTION IN LEAST SQUARES INTERFITSAL
     +       ----GUESS AGAIN ')                                       FITSAL
107 FORMAT (//,1X,'OPTION REDUNDANCY  - - -  EXPRESSION CHANGE ',      FITSAL
     +        'INDICATED')                                            FITSAL
                                                                        FITSAL
C.. HAVE WE IMPROVED ?                                                  FITSAL
      IF(ERROR.GE.ERRORH)GOTO 200                                       FITSAL
                                                                        FITSAL
C.. NEW LOW IN ERROR, SO RESET HOLDING OF PARAMETER VALUES              FITSAL
      DO 150 I=1,M3                                                     FITSAL
150   PARAM(I)=CORE(LOCB-1+I)                                           FITSAL
      DO 160 I=1,NB                                                     FITSAL
      DO 160 J=1,NB                                                     FITSAL
      IJ=J+NB*(I-1)                                                     FITSAL
160   AC(IJ)=CORE(LOCA-1+J+BDIM*(I-1))                                  FITSAL
      SUMC=SUMSQ                                                        FITSAL
                                                                        FITSAL
C.. UPDATE LOWEST ERROR SO FAR                                          FITSAL
      ERRORH=ERROR                                                      FITSAL
200   CONTINUE                                                          FITSAL
                                                                        FITSAL
```

```
C.. OUTPUT BEST PARAMETER VALUES FOUND AND ASSOCIATED A-MATRIX          FITSAL
C  >>>CHANEL CHANGE 5 TO 9!!                                           FITSAL
         WRITE(9,300)(PARAM(I),I=1,M3)                                FITSAL
         WRITE(9,300)SUMC                                             FITSAL
  300    FORMAT(1X,1P10E13.6)                                         FITSAL
         K1=1                                                         FITSAL
         DO 500 I=1,NB                                                FITSAL
         K2=K1+BDIM-1                                                 FITSAL
                                                                      FITSAL
         WRITE(9,300)(AC(K),K=K1,K2)                                  FITSAL
         K1=K2+1                                                      FITSAL
  500    CONTINUE                                                     FITSAL
 1000    CONTINUE                                                     FITSAL
                                                                      FITSAL
         REWIND IBCHN                                                 FITSAL
         CNTROL(8) =KNTR8                                             FITSAL
         CNTROL(10)=KNTR10                                            FITSAL
         CNTROL(11)=KNTR11                                            FITSAL
         CNTROL(12)=KNTR12                                            FITSAL
         CNTROL(19)=KNTR19                                            FITSAL
                                                                      FITSAL
         RETURN                                                       FITSAL
         END                                                          FITSAL
                                                                      FITSAL
      SUBROUTINE GAUSS(B,Z,MDIM,NDIM,BDIM,A)                          GAUSS
                                                                      GAUSS
C     SEEKS PARAMETER VALUES TO MINIMIZE:                             GAUSS
C                                                                     GAUSS
C        SUM [ W*(YOBS-YCALC) ] **2                                   GAUSS
C                                                                     GAUSS
C     BY SOLVING                                                      GAUSS
C                                                                     GAUSS
C        SUM [ W*DY/DB(1) * W*(YOBS-YCALC) ]                          GAUSS
C        SUM [ W*DY/DB(2) * W*(YOBS-YCALC) ]                          GAUSS
C        .                                                            GAUSS
C        .                                                            GAUSS
C        SUM [ W*DY/DB(JJ)*W*(YOBS-YCALC) ]                           GAUSS
C                                                                     GAUSS
C     FIRST ORDER SOLUTION IS:                                        GAUSS
C                                                                     GAUSS
C        BNEW(K) = BOLD(K) + [ SUM [ W*DY/DB(K) * W*DYDB(J) ]**(-1) * GAUSS
C                              SUM [ W*DY/DB(K) * W*(YOBS-YCALC) ]    GAUSS
C                                                                     GAUSS
C                                                                     GAUSS
C.. INPUT:                                                            GAUSS
C        Z(1,I)=OBSERVED VALUE OF Y FOR I-TH DATA POINT               GAUSS
C        Z(MDIM,I)=ERROR IN OBSERVED VALUE OF Y FOR I-TH DATA POINT   GAUSS
C        MDIM=1ST DIMENSION OF Z(   ,   )                             GAUSS
C        NDIM=2ND DIMENSION OF Z(   ,   )                             GAUSS
C        BDIM=DIMENSIONS OF A-ARRAY AND 1ST DIMENSION OF B-ARRAY      GAUSS
C        CNTROL(1)= # OF PARAMETERS BEING FITTED (ABS VAL)            GAUSS
C        CNTROL(6)=LIMIT ON # OF ITERATIONS                           GAUSS
C        CNTROL(7)=INTERMEDIATE OUTPUT PRINT FLAG                     GAUSS
C        CNTROL(9)=CONVERGENCE CRITERIA CONTROL                       GAUSS
C                 =1:                                                 GAUSS
C                 =2:                                                 GAUSS
C                 (MAY BE TEMPORARILY SET AT 3 FOR PASSING TO BTEST.FR) GAUSS
C        CNTROL(10)=PARAMETER VARIATION CONSTRAINT FLAG               GAUSS
```

```
C                = 0: UNCONSTRAINED PARAMETER CHANGES                    GAUSS
C                > 0: LIMIT ON PERCENTAGE CHANGE OF PARAMETERS           GAUSS
C                  (EXPRESSED IN UNITS OF TENS OF PERCENTS)              GAUSS
C       CNTROL(11)=CONTROL FOR OVERRIDING RESTRAINED CHANGE              GAUSS
C                   MECHANISM (WHEN JUMP TO STATEMENTS # 34, 28 OR 38)   GAUSS
C                = 1: OVERRIDING PERMITTED                               GAUSS
C                = 0: NO OVERRIDING                                      GAUSS
C       CNTROL(12)=OVERRIDE LIMIT                                        GAUSS
C                  [NEGATIVE VALUE SPECIFIES WRONG WAY MECHANISM]        GAUSS
C       CNTROL(13)= ?? (PARAMETER CHANGE OPTION ?)                       GAUSS
C       CNTROL(22)=INITIAL ENTRY FLAG                                    GAUSS
C                  =1: 1ST ENTRY                                         GAUSS
C                  =0: SUBSEQUENT ENTRY                                  GAUSS
C       SCONVG=CAUCHY CONVERGENCE CRITERION FOR SUM OF SQUARES           GAUSS
C       PCONVG=CAUCHY CONVERGENCE CRITERION FOR PARAMETERS               GAUSS
C       BCONVG=INCREASED VALUE OF PCONVG FOR SPECIAL CASES               GAUSS
C                                                                        GAUSS
C.. INTERMEDIATE:                                                        GAUSS
C       A(K,J)=SUM OVER DATA POINTS OF PRODUCT OF DY/DP(K) AND DY/DP(J)  GAUSS
C       B(J,1)=ESTIMATED VALUE OF J-TH PARAMETER                         GAUSS
C       B(J,2)=OLD ESTIMATED VALUE OF J-TH PARAMETER                     GAUSS
C       B(J,3)=SUM OVER DATA POINTS OF PRODUCT OF DEVIATION AND PARTIAL  GAUSS
C                DERIVATIVE OF Y WITH RESPECT TO K-TH PARAMETER          GAUSS
C       B(J,4)=WEIGHTED DERIVATIVE OF Y WITH RESPECT TO K-TH PARAMETER   GAUSS
C                                                                        GAUSS
C.. OUTPUT:                                                              GAUSS
C       B(J,1)=ESTIMATED VALUE OF J-TH PARAMETER                         GAUSS
C       A(J,I)=COVARIANCE COEFFICIENT FOR J-TH AND I-TH PARAMETERS       GAUSS
C       A(J,J)=VARIANCE COEFFICIENT FOR J-TH PARAMETER                   GAUSS
C       CNTROL(1) MAY BE CHANGED ON CALL TO YCOMP.FR                     GAUSS
C       CNTROL(10)=PARAMETER VARIATION CONSTRAINT FLAG                   GAUSS
C                          (MAY BE ALTERED BY THIS ROUTINE)              GAUSS
C          =-1: DON'T CHANGE A- AND B-ARRAYS; CONTINUE ON NEGLIGIBLE     GAUSS
C                          CHANGE IN SUM OF SQUARES TILL FACLIM HIT      GAUSS
C          =-2: DON'T CHANGE A- AND B-ARRAYS; WEIGHT SSQ BY NUMBER-JJ    GAUSS
C                          (IN SETUP.FR FROM FINALE.FR)                  GAUSS
C          =-3: DON'T CHANGE A- AND B-ARRAYS                             GAUSS
C       CNTROL(11)=0: NO MORE OVERRIDING OF RESTRAINED CHG MCHM PERMTD   GAUSS
C       CNTROL(12)=0: NO MORE OVERRIDING PERMITTED                       GAUSS
C       CNTROL(20)=NUMBER OF ITERATIONS USED                             GAUSS
C       CNTROL(21)=TERMINATION CODE                                      GAUSS
C       CNTROL(22)=INITIAL ENTRY FLAG (IS RESET TO 0 BY THIS ROUTINE)    GAUSS
                                                                         GAUSS
                                                                         GAUSS
        EXTERNAL BTEST                                                   GAUSS
        INTEGER CNTROL,BDIM                                              GAUSS
        COMMON/CNTROL/CNTROL(25)                                         GAUSS
        COMMON/CONVG/SCONVG,PCONVG,BCONVG                                GAUSS
        REAL A(BDIM,BDIM),B(BDIM,4),Z(MDIM,NDIM),S(24,6),P(24)           GAUSS
        LOGICAL L1,L2,L3,L4,L5                                           GAUSS
                                                                         GAUSS
C.. BINARY BITS FROM INTEGERS                                            GAUSS
C     BIN(K,J) = 0. : J-TH BIT OF K IS 0                                 GAUSS
C              = 1. : J-TH BIT OF K IS 1                                 GAUSS
        BIN(K,J)=0.5-0.5*(-1.)**(K/2**(J-1))                             GAUSS
                                                                         GAUSS
C.. SET CNTROL(22)=0 TO INDICATE COMPLETION OF INITIAL ENTRY             GAUSS
D       WRITE(6,990)                                                     GAUSS
```

```
  990     FORMAT(/,1X,'ENTERED MODULE GAUSS')                              GAUSS
          IF(CNTROL(22).EQ.0)GOTO 5                                        GAUSS
                                                                           GAUSS
C.. SET DETERM=1. ON INITIAL ENTRY                                         GAUSS
          DETERM=1.                                                        GAUSS
          CNTROL(22)=0                                                     GAUSS
     2    FORMAT(/,'CYCLE    SUM OF SQUARES       **********',GAUSS
      +'********** B(J) PARAMETERS  **********',/)GAUSS
                                                                           GAUSS
     5    NN=0                                                             GAUSS
          NOR=0                                                            GAUSS
          NWW=0                                                            GAUSS
          NWFLAG=0                                                         GAUSS
          NVSTORE=0                                                        GAUSS
          PCHGSS=0.                                                        GAUSS
                                                                           GAUSS
C.. IS RESTRAINED CHANGE MECHANISM ACTIVATED ?                             GAUSS
          IF(CNTROL(10).LE.0)GOTO 7                                        GAUSS
                                                                           GAUSS
C.. INITIAL VALUE OF VARIATIONAL FACTOR                                    GAUSS
         FAC=0.1*FLOAT(CNTROL(10))                                         GAUSS
                                                                           GAUSS
C.. LIMIT ON PARAMETER VARIATIONS                                          GAUSS
          FACLIM=CNTROL(10)                                                GAUSS
          GOTO 8                                                           GAUSS
     7    FAC=1.0                                                          GAUSS
          FACLIM=FAC                                                       GAUSS
     8    OLFAC=0.                                                         GAUSS
          JJ=IABS(CNTROL(1))        ! # PARAMETERS BEING FITTED            GAUSS
          LIMIT=CNTROL(6)           ! LIMIT ON # OF ITERATIONS             GAUSS
          L=CNTROL(7)               ! INTERMEDIATE OUTPUT PRINT FLAG       GAUSS
          L1=.FALSE.                                                       GAUSS
          L2=.FALSE.                                                       GAUSS
          L3=.FALSE.                                                       GAUSS
          L4=.FALSE.                                                       GAUSS
          L5=.FALSE.                                                       GAUSS
          IF(BIN(L,1).EQ.1.)L1=.TRUE.                                      GAUSS
          IF(BIN(L,2).EQ.1.)L2=.TRUE.                                      GAUSS
          IF(BIN(L,3).EQ.1.)L3=.TRUE.                                      GAUSS
          IF(BIN(L,4).EQ.1.)L4=.TRUE.                                      GAUSS
          IF(BIN(L,5).EQ.1.)L5=.TRUE.                                      GAUSS
          CNTROL(20)=NN             ! # OF ITERATIONS                      GAUSS
                                                                           GAUSS
C.. TERMINATION CODE IS CONTINUALLY UP-DATED BY THIS ROUTINE)              GAUSS
          CNTROL(21)=69                                                    GAUSS
                                                                           GAUSS
                                                                           GAUSS
C.. MAKE 2-ND COPY OF INPUT GUESSES                                        GAUSS
          DO 3 J=1,JJ                                                      GAUSS
  3       B(J,2)=B(J,1)                                                    GAUSS
C        WRITE(2,*)'B(J,2)= ',B(J,2)                                       GAUSS
          SCALE=0.5                                                        GAUSS
          MARK10=CNTROL(10)         ! PARAMETER VARIATION CONSTRAINT FLAG  GAUSS
C          PRINT *,'CNTROL =',(CNTROL(J),J=1,19)                           GAUSS
                                                                           GAUSS
C.. COMPUTE PARTIAL DERIVATIVES AND COMPUTE A- & B-MATRICES                GAUSS
    10    CALL SETUP(B,Z,A,SUMSQ,MDIM,NDIM,BDIM)                           GAUSS
                                                                           GAUSS
```

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C.. ARE THE EQUATIONS SINGULAR ?                                        GAUSS
      IF(DETERM.NE.0.)GOTO 12                                           GAUSS
      WRITE(2,13)                                                       GAUSS
   13 FORMAT(/,' THE FOLLOWING NORMAL EQUATIONS ARE SINGULAR')          GAUSS
      CALL DMPMAT(CNTROL,BDIM,A,B(1,3))                                 GAUSS
                                                                        GAUSS
C.. TERMINATE BECAUSE EQUATIONS ARE SINGULAR                            GAUSS
      CNTROL(21)=4                                                      GAUSS
      RETURN                                                            GAUSS
                                                                        GAUSS
C.. IF NOT CHANGING A- & B-ARRAYS AND PRINT WANTED OF RESTRAINED        GAUSS
C      CHANGE MECHANISM, GOTO 21                                        GAUSS
   12 IF(CNTROL(10).LE.-1.AND.L4)GOTO 21                                GAUSS
      IF(CNTROL(10).LE.-1)GOTO 25                                       GAUSS
      IF(L3)CALL DMPMAT(CNTROL,BDIM,A,B(1,3))                           GAUSS
                                                                        GAUSS
C.. IF ON INITIAL ITERATION:                                            GAUSS
   21 IF(NN.EQ.0)SQMIN=SUMSQ                                            GAUSS
                                                                        GAUSS
C.. IF PRINT WANTED OF SUMSQ & PARM VALS                                GAUSS
      IF(L2)WRITE(2,2)                                                  GAUSS
      IF(L2)WRITE(2,14)NN,SUMSQ,(B(J,1),J=1,JJ)                         GAUSS
   14 FORMAT(1HO I2,1P2E21.7,4E15.7/(E45.7,4E15.7))                     GAUSS
                                                                        GAUSS
C.. IF NOT CHANGING A- & B-ARRAYS, GO AND TEST CONVERGENCE              GAUSS
      IF(CNTROL(10).LE.-1)GOTO 25                                       GAUSS
C      IF(CNTROL(20).LE.LIMIT)GOTO 20                                   GAUSS
CC.. TERmINATE BECAUSE HIT LIMIT ON NUMBER OF ITERATIONS                GAUSS
C      CNTROL(21)=3                                                     GAUSS
C      RETURN                                                           GAUSS
                                                                        GAUSS
C   20  CONTINUE                                                        GAUSS
      IF(JJ.NE.1)GOTO 16                                                GAUSS
      B(1,3)=B(1,3)/A(1,1)                                              GAUSS
      A(1,1)=1./A(1,1)                                                  GAUSS
      GOTO 160                                                          GAUSS
                                                                        GAUSS
C.. INVERT A-MATRIX & UP-DATE 3-RD COLUMN OF B-MATRIX                   GAUSS
C.. NOTE: ONLY USING M=1 ROW OF B-ARRAY                                 GAUSS
   16 CONTINUE                                                          GAUSS
      PPP=1.                                                            GAUSS
      DO 4444 I88=1,JJ                                                  GAUSS
      PPP=PPP*A(I88,I88)                                                GAUSS
 4444 CONTINUE                                                          GAUSS
      WRITE(2,994)PPP                                                   GAUSS
  994 FORMAT(1X,'PPP=',1PE15.6)                                         GAUSS
      CALL MATINV(A,JJ,B(1,3),1,DETERM,BDIM)                            GAUSS
      WRITE(2,995)DETERM                                                GAUSS
  995 FORMAT(1X,'DETERM=',1PE15.6)                                      GAUSS
C     DO 5555 I88=1,BDIM                                                GAUSS
C     DO 5555 J88=1,BDIM                                                GAUSS
C5555 A(I88,J88)=SNGL(AAA(I88,J88))                                     GAUSS
                                                                        GAUSS
  160 CONTINUE                                                          GAUSS
      IF(CNTROL(20).LE.LIMIT)GOTO 20                                    GAUSS
C.. TERMINATE BECAUSE HIT LIMIT ON NUMBER OF ITERATIONS                 GAUSS
      CNTROL(21)=3                                                      GAUSS
      RETURN                                                            GAUSS
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C.. IF NOT PRINTING NORMAL EQNS, GOTO 17                                GAUSS
   20     IF(.NOT.L3)GOTO 17                                            GAUSS
                                                                        GAUSS
C.. HOLD TERMINATION CODE                                               GAUSS
          IHOLD=CNTROL(21)                                              GAUSS
                                                                        GAUSS
C.. TEMPORARILY SET TERMINATION CODE AT 70                              GAUSS
C         (IN CASE YCOMP.FR NEEDS TO KNOW SOURCE OF CALL)               GAUSS
C         (NO NEED TO DO THIS IF NOT CALLING DMPMAT.FR)                 GAUSS
          CNTROL(21)=70                                                 GAUSS
          CALL DMPMAT(CNTROL,BDIM,A,B(1,3))                             GAUSS
                                                                        GAUSS
C.. RESTORE TERMINATION CODE                                            GAUSS
          CNTROL(21)=IHOLD                                              GAUSS
                                                                        GAUSS
C.. UP-DATE ITERATION COUNTER                                           GAUSS
   17     NN=NN+1                                                       GAUSS
          WRITE(6,996)NN                                                GAUSS
  996     FORMAT(10X,'ITER # =',I3)                                     GAUSS
          CNTROL(20)=NN           ! ITERATION COUNTER                   GAUSS
          RESCAL=0.5                                                    GAUSS
          IF(DETERM.EQ.0.)GOTO 10                                       GAUSS
                                                                        GAUSS
C.. LOAD S(I,1-4 & 6)                                                   GAUSS
          DO 11 I=1,JJ                                                  GAUSS
          S(I,4)=-1.                                                    GAUSS
          IF(B(I,3).LT.0..AND.B(I,1).LT.0..OR.B(I,3).GT.0..AND.         GAUSS
     +B(I,1).GT.0.)S(I,4)=1.                                            GAUSS
          S(I,1)=B(I,1)                                                 GAUSS
          S(I,3)=B(I,3)                                                 GAUSS
          S(I,6)=S(I,4)                                                 GAUSS
   11     S(I,2)=(FAC-OLFAC)*S(I,1)*S(I,4)                              GAUSS
                                                                        GAUSS
C.. IF PRINTING NORMAL EQNS, ALSO PRINT S-MATRIX                        GAUSS
          IF(L3)WRITE(2,23)((S(J,I),I=1,4),J=1,JJ)                      GAUSS
   23     FORMAT (/,' S PARAMETERS ',//(1P4E12.4))                      GAUSS
                                                                        GAUSS
C.. TEST FOR CONVERGENCE & UP-DATE PARM ESTIMATES IF CONVERGED          GAUSS
   40     CALL BTEST(CNTROL,B,BDIM)                                     GAUSS
                                                                        GAUSS
C.. HAVE WE CONVERGED ?                                                 GAUSS
          IF(CNTROL(21).NE.1)GOTO 45                                    GAUSS
   36     IF((CNTROL(10).EQ.-1).AND.(FAC.NE.FACLIM))GOTO 9              GAUSS
          IF(CNTROL(10).GE.0.AND.NVSTORE.NE.0)GOTO 2212                 GAUSS
                                                                        GAUSS
C.. TERMINATION, CAUCHY CONVERGENCE OF PARAMETERS                       GAUSS
          IF(CNTROL(10).NE.-1)RETURN                                    GAUSS
          CNTROL(21)=5   !NO SSQ RED; ISSUE 'GUESS AGAIN' REQ. IF NOR   GAUSS
                                                                        GAUSS
C.. ARE OVERRIDES PERMITTED ?                                           GAUSS
          IF(CNTROL(12).LE.0)GOTO 18                                    GAUSS
                                                                        GAUSS
C.. UPDATE COUNT OF NUMBER OF OVERRIDES                                 GAUSS
          NOR=NOR+1                                                     GAUSS
          WRITE(6,345)NOR                                               GAUSS
  345     FORMAT(10X,'OVERRIDE(12): NOR=',I3)                           GAUSS
          IF(L2)WRITE(2,62)NOR,SQMIN                                    GAUSS
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   62     FORMAT (' NO CONVERGENCE IN SCALING INTERVAL. OVERRIDE ',      GAUSS
     +           'MECHANISM NOW OPERABLE - OVERRIDE ',I3,                GAUSS
     +           ' SUM OF SQUARES MINIMUM IS',1PE14.6)                   GAUSS
                                                                         GAUSS
C.. HAVE WE EXCEEDED PERMISSIBLE NUMBER OF OVERRIDES ?                   GAUSS
          IF(NOR.GT.CNTROL(12))GOTO 57                                   GAUSS
                                                                         GAUSS
C.. ARE WE ON FIRST OVERRIDE ?                                           GAUSS
          IF(NOR.NE.1)GOTO 38                                            GAUSS
                                                                         GAUSS
C.. ON FIRST OVERRIDE, SO LOAD S(J,5) & P(J) WITH CURRENT VARIANCE       GAUSS
C     COEFFICIENTS AND PARAMETER ESTIMATES                               GAUSS
          DO 58 J=1,JJ                                                   GAUSS
          S(J,5)=A(J,J)                                                  GAUSS
   58     P(J)=S(J,1)                                                    GAUSS
          ICYC=CNTROL(20)-1                                              GAUSS
          GOTO 38                                                        GAUSS
                                                                         GAUSS
C.. EXCEEDED OVERRIDE LIMIT, SO WRAP-UP AND GET OUT                      GAUSS
C.. UP-DATE VARIANCE COEFFICIENTS AND PARAMETER ESTIMATES                GAUSS
   57     DO 59 J=1,JJ                                                  GAUSS
          A(J,J)=S(J,5)                                                  GAUSS
   59     B(J,1)=P(J)                                                    GAUSS
          NOR=NOR-1                                                      GAUSS
          IF(L2)WRITE(2,60)NOR,ICYC                                      GAUSS
   60     FORMAT(/,' AFTER 'I3' OVERRIDES    REFERENCE ITERATION ',I4)   GAUSS
          RETURN                                                         GAUSS
   18     IF(CNTROL(12).EQ.0)GOTO 2212                                   GAUSS
                                                                         GAUSS
C.. NEGATIVE CNTROL(12) SPECIFIES WRONG WAY MECHANISM                    GAUSS
          IF(L2)WRITE(2,29)SQMIN                                         GAUSS
   29     FORMAT (' NO CONVERGENCE IN SCALING INTERVAL. WRONGWAY ',      GAUSS
     +           'MECHANISM NOW OPERABLE  SUM OF SQUARES MINIMUM IS ',   GAUSS
     +           1PE14.6)                                                GAUSS
          IF(NWW.NE.0)GOTO 299                                           GAUSS
          DO 290 J=1,JJ                                                  GAUSS
          S(J,5)=A(J,J)                                                  GAUSS
  290     P(J)=S(J,1)                                                    GAUSS
          ICYC=CNTROL(20)-1                                              GAUSS
  299     SMAX=ABS(S(1,3)/S(1,1))                                        GAUSS
          DO 64 J=2,JJ                                                   GAUSS
          IF(ABS(S(J,3)/S(J,1)).GT.SMAX)SMAX=ABS(S(J,3)/S(J,1))          GAUSS
   64     CONTINUE                                                       GAUSS
                                                                         GAUSS
C.. UP-DATE PARAMETER ESTIMATES                                          GAUSS
          DO 33 J=1,JJ                                                   GAUSS
          SFRAC=ABS(S(J,3)/(SMAX*S(J,1)))                                GAUSS
   33     B(J,1)=S(J,1)-0.05*S(J,6)*S(J,1)*SFRAC                         GAUSS
          CNTROL(10)=-1                                                  GAUSS
          IF(NWW.GE.IABS(CNTROL(12)))GOTO 22                             GAUSS
          NWW=NWW+1                                                      GAUSS
          NWFLAG=1                                                       GAUSS
          GOTO 10                                                        GAUSS
                                                                         GAUSS
C.. UP-DATE VARIANCE COEFFICIENTS AND PARAMETER ESTIMATES                GAUSS
   22     DO 220 J=1,JJ                                                  GAUSS
          A(J,J)=S(J,5)                                                  GAUSS
  220     B(J,1)=P(J)                                                    GAUSS
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      IF(L2)WRITE(2,221)ICYC                                          GAUSS
  221 FORMAT (/,' WRONGWAY LIMIT EXCEEDED',                           GAUSS
     +        '     REFERENCE ITERATION',I4)                         GAUSS
 2212 IF(CNTROL(11).EQ.0.AND.CNTROL(12).EQ.0)GOTO 15          ! 11    GAUSS
      IF(CNTROL(11).EQ.0)RETURN                               ! 11    GAUSS
      IF(CNTROL(21).EQ.1.OR.CNTROL(21).EQ.2)CNTROL(21)=69             GAUSS
      IF(NVSTORE.NE.0.AND.SQMIN.GE.PCHGSS)GOTO 2219                   GAUSS
      CON13=CNTROL(13)                          ! 13                  GAUSS
      NUMBEE=JJ                                                       GAUSS
      DO 2214 J=1,JJ                                                  GAUSS
C     CON13=CNTROL(13)                            ! 13                GAUSS
C     NUMBEE=JJ                                                       GAUSS
      S(J,5)=A(J,J)                                                   GAUSS
      IF(CNTROL(12).GE.0.OR.CNTROL(21).EQ.69)P(J)=S(J,1)              GAUSS
 2214 CONTINUE                                                        GAUSS
                                                                      GAUSS
C.. WORDING OF FOLLOWING STATEMENT CHANGED ************              GAUSS
 2219 IF(SQMIN.NE.PCHGSS)GUTO 223                                     GAUSS
      WRITE(2,226)                                                    GAUSS
  226 FORMAT(/,' PARAMETER CHANGE OPTION UNAVAILING')                 GAUSS
      WRITE(10,226)                                                   GAUSS
      CNTROL(21)=0                                                    GAUSS
      NVSTORE=YCOMP(NDIM+1,B,Z,MDIM,NDIM,BDIM)                        GAUSS
                                                                      GAUSS
C.. NOTE: CALL TO YCOMP WITH FIRST ARG= NDIM+1 CAN CHANGE CNTROL(1)   GAUSS
      IF(NVSTORE.NE.0)GOTO 2265                                       GAUSS
      CNTROL(13)=CON13                          ! 13                  GAUSS
      CNTROL(1)=NUMBEE                                                GAUSS
      JJ=NUMBEE                                                       GAUSS
      DO 2262 J=1,NUMBEE                                              GAUSS
C     CNTROL(13)=CON13                            ! 13                GAUSS
C     CNTROL(1)=NUMBEE                                                GAUSS
C     JJ=NUMBEE                                                       GAUSS
      A(J,J)=S(J,5)                                                   GAUSS
 2262 B(J,1)=P(J)                                                     GAUSS
                                                                      GAUSS
C.. TERMINATE BECAUSE OF OPTION REDUNDANCY                            GAUSS
      RETURN                                                          GAUSS
                                                                      GAUSS
 2265 NVSTORE=0                                                       GAUSS
      JJ=IABS(CNTROL(1))                                              GAUSS
      CNTROL(11)=0                              ! 11                  GAUSS
      CNTROL(12)=0                                                    GAUSS
      GOTO 28                                                         GAUSS
                                                                      GAUSS
  223 PCHGSS=SQMIN                                                    GAUSS
      NVSTORE=YCOMP(NDIM+1,B,Z,MDIM,NDIM,BDIM)                        GAUSS
      NVAB=IABS(NVSTORE)                                              GAUSS
      NEWNV=IABS(CNTROL(1))                                           GAUSS
      WRITE(2,225)NVAB,NEWNV                                          GAUSS
  225 FORMAT(/,1X,'THE NUMBER OF LSTSQ PARAMETERS HAS BEEN ',         GAUSS
     +       'CHANGED FROM',I3,' TO',I3)                              GAUSS
      WRITE(6,225)NVAR,NEWNV                                          GAUSS
      NN=CNTROL(20)                                                   GAUSS
      JJ=IABS(CNTROL(1))                                              GAUSS
      GOTO 28                                                         GAUSS
                                                                      GAUSS
C.. UP-DATE PARAMETER ESTIMATES                                       GAUSS
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   15     DO 1 J=1,JJ                                                    GAUSS
    1     B(J,1)=S(J,1)                                                  GAUSS
          RETURN                                                         GAUSS
                                                                         GAUSS
   45     IF((MARK10.EQ.0).OR.(CNTROL(10).EQ.-1))GOTO 46                 GAUSS
                                                                         GAUSS
          DO 47 J=1,JJ                                                   GAUSS
          IF(ABS(B(J,3)).LE.ABS(FAC*S(J,1)))GOTO 48                      GAUSS
          B(J,3)=S(J,4)*FAC*S(J,1)                                       GAUSS
          IF(ABS(B(J,3)).EQ.ABS(S(J,1)).AND.S(J,4).EQ.-1.)               GAUSS
     +B(J,3)=B(J,3)+SIGN(SCONVG,S(J,1))    ! ********* 1.0E-12 ********  GAUSS
          GOTO 47                                                        GAUSS
   48     S(J,2)=B(J,3)                                                  GAUSS
          S(J,4)=0.                                                      GAUSS
   47     CONTINUE                                                       GAUSS
                                                                         GAUSS
C.. IS S(J,4)=4 FOR ALL J ?                                              GAUSS
          DO 52 J=1,JJ                                                   GAUSS
          IF(S(J,4).NE.0.)GOTO 46                                        GAUSS
   52     CONTINUE                                                       GAUSS
                                                                         GAUSS
C.. IF S(J,4)=0 FOR ALL J, THEN SET FAC=FACLIM                           GAUSS
          FAC=FACLIM                                                     GAUSS
                                                                         GAUSS
C.. UP-DATE PARAMETER ESTIMATES                                          GAUSS
   46     DO 50 J=1,JJ                                                   GAUSS
   50     B(J,1)=(B(J,2)+B(J,3))                                         GAUSS
          IF(CNTROL(10).NE.-1)CNTROL(10)=-3                              GAUSS
          GOTO 10                                                        GAUSS
                                                                         GAUSS
C.. TEST CAUCHY CONVERGENCE OF SUM OF SQUARES                            GAUSS
C     WE HAVE CONVERGED WHEN NEW SUMSQ REDUCES OLD SQMIN BY A FRACTION   GAUSS
C     OF SCONVG OR LESS                                                  GAUSS
   25     TEST=ABS((SUMSQ-SQMIN)/SQMIN)                                  GAUSS
          IF(TEST.GT.SCONVG)GOTO 30                                      GAUSS
          CNTROL(21)=2                                                   GAUSS
          IF((CNTROL(10).EQ.-1).AND.(FAC.NE.FACLIM))GOTO 9               GAUSS
          WRITE(2,251)                                                   GAUSS
  251     FORMAT(/,' NEGLIGIBLE CHANGE IN SUM OF SQUARES')               GAUSS
C.. TERMINATE BECAUSE OF NEGLIGIBLE CHANGE IN SUM OF SQUARES             GAUSS
          IF(NVSTORE.EQ.0)RETURN                                         GAUSS
                                                                         GAUSS
          GOTO 2212                                                      GAUSS
                                                                         GAUSS
    9     RESCAL=0.5                                                     GAUSS
                                                                         GAUSS
C.. SET TERMINATION CODE TO 89                                           GAUSS
          CNTROL(21)=89                                                  GAUSS
                                                                         GAUSS
C.. STORE OLD VALUE OF FAC                                               GAUSS
          OLFAC=FAC                                                      GAUSS
                                                                         GAUSS
C.. INCREASE VARIATIONAL FACTOR (BUT NOT GREATER THAN FACLIM)            GAUSS
          FAC=2.*FAC                                                     GAUSS
          IF(FAC.GT.FACLIM)FAC=FACLIM                                    GAUSS
          CNTROL(10)=MARK10                                              GAUSS
                                                                         GAUSS
C.. UP-DATE ITERATION COUNTER                                            GAUSS
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      NN=NN+1                                                          GAUSS
      PRINT *,'ITER # =',NN                                            GAUSS
      DO 41 J=1,JJ                                                     GAUSS
      B(J,3)=S(J,3)                                                    GAUSS
41    S(J,2)=(FAC-OLFAC)*S(J,1)*S(J,4)                                 GAUSS
      GOTO 45                                                          GAUSS
                                                                       GAUSS
30    IF(SUMSQ.LT.SQMIN)GOTO 34                                        GAUSS
                                                                       GAUSS
C.. WORDING OF FOLLOWING STATEMENT CHANGED *********                   GAUSS
      IF(NWFLAG.LE.0)GOTO 71                                           GAUSS
      NWFLAG=0                                                         GAUSS
      GOTO 38                                                          GAUSS
                                                                       GAUSS
71    CNTROL(10)=-1                                                    GAUSS
      DIFFAC=FAC-OLFAC                                                 GAUSS
      SCAFAC=RESCAL*DIFFAC                                             GAUSS
      RESCAL=SCALE*RESCAL                                              GAUSS
      IF((MARK10.NE.0).OR..NOT.L4)GOTO 24                              GAUSS
                                                                       GAUSS
      DO 27 J=1,JJ                                                     GAUSS
27    B(J,3)=SCALE*B(J,3)                                              GAUSS
                                                                       GAUSS
C.. TEST FOR CONVERGENCE & UP-DATE PARM ESTIMATES IF CONVERGED         GAUSS
      CALL BTEST(CNTROL,B,BDIM)                                        GAUSS
                                                                       GAUSS
C.. WORDING OF FOLLOWING STATEMENT CHANGED *********                   GAUSS
C.. HAVE WE CONVERGED ?                                                GAUSS
      IF(CNTROL(21).NE.1)GOTO 39                                       GAUSS
      IF(L4)WRITE(2,42)                                                GAUSS
42    FORMAT(/,' PARTITION LESS THAN MESH LIMIT - - -                  GAUSS
     +       RECYCLE RESTRAINT MECHANISM')                             GAUSS
      GOTO 36                                                          GAUSS
39    IF(L4)WRITE(2,26)SCAFAC,OLFAC                                    GAUSS
26    FORMAT (/,' NO REDUCTION IN SUM OF SQUARES. RESCALE ',           GAUSS
     +       'PARAMETERS ',//,' RESTRAINED CHANGE MECHANISM SET ',     GAUSS
     +       'AT (',E11.4,'+',F7.4,') TIMES THE PREDICTED LSTSQ',      GAUSS
     +       ' CORRECTION.')                                           GAUSS
      GOTO 46                                                          GAUSS
                                                                       GAUSS
24    DO 31 J=1,JJ                                                    GAUSS
      S(J,2)=SCALE*S(J,2)                                              GAUSS
      B(J,3)=S(J,2)                                                    GAUSS
31    CONTINUE                                                         GAUSS
                                                                       GAUSS
C.. HOLD CNTROL(9), WHICH SPECIFIES THE DEPENDENT VARIABLE             GAUSS
      INTER=CNTROL(9)                                                  GAUSS
                                                                       GAUSS
C.. IF OLFAC=0, DON'T RELAX CONVERGENCE CRITERION                      GAUSS
      IF(OLFAC.EQ.0.)GOTO 61                                           GAUSS
                                                                       GAUSS
C.. TEMPORARILY SET CNTROL(9) TO 3, THUS RELAXING CONVERGENCE CRITERION GAUSS
C           & BY-PASSING PARM ESTIMATE UP-DATE                         GAUSS
      CNTROL(9)=3                                                      GAUSS
                                                                       GAUSS
C.. TEST FOR CONVERGENCE                                               GAUSS
61    CALL BTEST(CNTROL,B,BDIM)                                        GAUSS
                                                                       GAUSS
```

```
C.. RESTORE CNTROL(9)                                                    GAUSS
      CNTROL(9)=INTER                                                    GAUSS
      DO 37 J=1,JJ                                                       GAUSS
      IF(ABS(S(J,3)).GT.FAC*S(J,1))B(J,3)=S(J,2)+OLFAC*S(J,1)*S(J,4)     GAUSS
 37   CONTINUE                                                           GAUSS
                                                                         GAUSS
C.. WORDING OF FOLLOWING STATEMENT CHANGED *******                       GAUSS
      IF(CNTROL(21).NE.1)GOTO 44                                         GAUSS
      IF(L4)WRITE(2,42)                                                  GAUSS
      GOTO 38                                                            GAUSS
                                                                         GAUSS
 44   IF(L4)WRITE(2,63)SCAFAC,OLFAC                                      GAUSS
 63   FORMAT (/,' NO REDUCTION IN SUM OF SQUARES. RESCALE ',             GAUSS
     +        'PARAMETERS ',//,' RESTRAINED CHANGE MECHANISM SET',       GAUSS
     +        'AT (',E11.4,'+',F7.4,') TIMES THE VALUE OF THE ',         GAUSS
     +        'ORIGINAL PARAMETER')                                      GAUSS
      GOTO 40                                                            GAUSS
 34   SQMIN=SUMSQ                                                        GAUSS
      WRITE(2,997)SQMIN                                                  GAUSS
997   FORMAT(1X,'NEW SQMIN=',1PE15.6)                                    GAUSS
      NOR=0                                                              GAUSS
 28   NWW=0                                                              GAUSS
      NWFLAG=0                                                           GAUSS
 38   IF(MARK10.GE.1)FAC=0.1*FLOAT(MARK10)                               GAUSS
      NN=CNTROL(20)                                                      GAUSS
      OLFAC=0.                                                           GAUSS
                                                                         GAUSS
C.. UP-DATE 2ND COPY OF PARAMETER ESTIMATES                              GAUSS
      DO 35 J=1,JJ                                                       GAUSS
 35   B(J,2)=B(J,1)                                                      GAUSS
                                                                         GAUSS
C.. WORDING OF FOLLOWING STATEMENT CHANGED *********                     GAUSS
      IF(NVSTORE.NE.0.AND.CNTROL(11).EQ.1)GOTO 231            ! 11       GAUSS
      CNTROL(10)=MARK10                                                  GAUSS
      GOTO 10                                                            GAUSS
                                                                         GAUSS
231   CNTROL(10)=0                                                       GAUSS
      GOTO 10                                                            GAUSS
                                                                         GAUSS
      END                                                                GAUSS
                                                                         GAUSS
     SUBROUTINE SETUP(B,Z,A,SUMSQ,MDIM,NDIM,BDIM)                        SETUP
                                                                         SETUP
C    CALLED BY GAUSS.FR & FINALE.FR                                      SETUP
C.. INPUT:                                                               SETUP
C       CNTROL(1) = TOTAL # PARAMETERS (ABS VAL)                         SETUP
C       CNTROL(3) = # DATA POINTS (ABS VAL)                              SETUP
C       CNTROL(8) = I.D. # FOR WEIGHTING FCN SELECTED                    SETUP
C       CNTROL(10) = PARAMETER CHANGE CONSTRAINT CONTROL                 SETUP
C          = -3: DON'T CHANGE A- & B-ARRAYS                              SETUP
C          = -2: DON'T CHANGE A- & B-ARRAYS, WEIGHT SSQ BY NUMBER-JJ     SETUP
C          = -1: DON'T CHANGE A- & B-ARRAYS                              SETUP
C          =  0: UNCONSTRAINED CHANGE PERMITTED                          SETUP
C          >  0: LIMIT ON PERCENTAGE CHANGE PERMITTED                    SETUP
C       Z(1,N)=OBSERVED VALUE OF Y FOR N-TH DATA POINT                   SETUP
C       Z(MDIM,N)=ERROR IN OBSERVED VALUE OF Y FOR N-TH DATA POINT       SETUP
C       MDIM=1ST DIMENSION OF Z(   ,   )                                 SETUP
C       NDIM=2ND DIMENSION OF Z(   ,   )                                 SETUP
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C       BDIM=DIMENSIONS OF A-ARRAY AND 1ST DIMENSION OF B-ARRAY          SETUP
C                                                                        SETUP
C.. OUTPUT:                                                              SETUP
C       B(K,4)=WEIGHTED DERIVATIVE OF Y WITH RESPECT TO K-TH PARAMETER   SETUP
C       B(K,3)=SUM OVER DATA POINTS OF PRODUCT OF DEVIATION AND PARTIAL  SETUP
C              DERIVATIVE OF Y WITH RESPECT TO K-TH PARAMETER            SETUP
C       A(K,J)=SUM OVER DATA POINTS OF PRODUCT OF DY/DB(K) AND DY/DB(J)  SETUP
C       SUMSQ=VARIANCE FOR THE FIT                                       SETUP
                                                                         SETUP
                                                                         SETUP
        INTEGER CNTROL,BDIM                                              SETUP
        COMMON/CNTROL/CNTROL(25)                                         SETUP
        REAL A(BDIM,BDIM),B(BDIM,4),Z(MDIM,NDIM)                         SETUP
C       WRITE(2,*)'CNTROL=',(CNTROL(I),I=1,25)                           SETUP
C       WRITE(2,*)'MDIM,NDIM,BDIM=',MDIM,NDIM,BDIM                       SETUP
                                                                         SETUP
        JJ=IABS(CNTROL(1))      ! # PARAMETERS BEING FITTED              SETUP
        LL=CNTROL(8)    ! WEIGHTING FCN INDEX                            SETUP
C       WRITE(2,*)'ENTERED SETUP, LL=',LL                                SETUP
C       WRITE(2,*)                                                       SETUP
C.. IF CNTROL(10) < 0, DON'T CHANGE A- AND B-ARRAYS                      SETUP
        IF(CNTROL(10).LE.-1)GOTO 6                                       SETUP
        DO 5 J=1,JJ                                                      SETUP
        B(J,3)=0.                                                        SETUP
        DO 5 K=1,JJ                                                      SETUP
    5   A(J,K)=0.                                                        SETUP
    6   NUMBER=IABS(CNTROL(3))      ! # DATA POINTS (ABS VAL)            SETUP
C.. INITIALIZE SSQ                                                       SETUP
        SUMSQ=0.                                                         SETUP
C.. HOLD TERMINATION CODE                                                SETUP
        IHOLD=CNTROL(21)                                                 SETUP
C.. TEMPORARILY SET TERMINATION CODE TO 68  (IN CASE YCOMP.FR NEEDS TO   SETUP
C                               IDENTIFY THE FIRST CALL FROM SETUP.FR)   SETUP
        CNTROL(21)=68                                                    SETUP
        ZERO=1./FLOAT(NUMBER-JJ)                                         SETUP
        IF(CNTROL(10).EQ.-2)ZERO=1.                                      SETUP
                                                                         SETUP
C.. LOOP OVER DATA POINTS                                                SETUP
        DO 15 N=1,NUMBER                                                 SETUP
                                                                         SETUP
C       WRITE(2,*)'**** N= ',N                                           SETUP
                                                                         SETUP
C.. COMPUTE Y FOR N-TH DATA POINT, USING THE OBSERVED VALUES OF THE      SETUP
C    NVARS-1 INDEPENDENT VARIABLES                                       SETUP
C    AND THE INPUTTED VALUES OF THE CNTROL(2) PARAMETERS                 SETUP
C       WRITE(2,*)'N,MDIM,NDIM,BDIM=',N,MDIM,NDIM,BDIM                   SETUP
C       WRITE(2,*)'CALLING YCOMP, LL=',LL                                SETUP
                                                                         SETUP
        YC=YCOMP(N,B,Z,MDIM,NDIM,BDIM)                                   SETUP
                                                                         SETUP
C       WRITE(2,*)'RETURNED FROM YCOMP, LL=',LL                          SETUP
C.. RESTORE TERMINATION CODE                                             SETUP
        CNTROL(21)=IHOLD                                                 SETUP
C       IF(NUMBER.NE.IABS(CNTROL(3)))GOTO 6     ; ????????               SETUP
C.. NOTE OBSERVED VALUE OF Y FOR N-TH DATA POINT                         SETUP
        ZN=Z(1,N)                                                        SETUP
C.. COMPUTE DEVIATION FOR N-TH DATA POINT                                SETUP
        DELY=ZN-YC                                                       SETUP
```

```
                                                                      SETUP
C       WRITE(2,*)'N,ZN,YC=',N,ZN,YC                                  SETUP
                                                                      SETUP
C.. BRANCH ACCORDING TO WEIGHTING FCN SELECTED                        SETUP
        W=1.                                                          SETUP
C       WRITE(2,*)'LL=',LL                                            SETUP
        GOTO (50,42,43,44,45,46,47,48),LL                             SETUP
   42   W=1./ZN                                                       SETUP
        GOTO 50                                                       SETUP
   43   W=1./YC                                                       SETUP
        GOTO 50                                                       SETUP
   44   W=ZN                                                          SETUP
        GOTO 50                                                       SETUP
   45   W=YC                                                          SETUP
        GOTO 50                                                       SETUP
   46   W=1./Z(MDIM,N)                                                SETUP
        GOTO 50                                                       SETUP
   47   W=Z(MDIM,N)                                                   SETUP
        GOTO 50                                                       SETUP
   48   IF (ABS(ZN).GT.ABS(YC)) W=ZN                                  SETUP
        IF (ABS(YC).GE.ABS(ZN)) W=YC                                  SETUP
                                                                      SETUP
   50   DELY=DELY*W                                                   SETUP
                                                                      SETUP
C       WRITE(2,*)'W=',W                                              SETUP
                                                                      SETUP
                                                                      SETUP
C.. COMPUTE WEIGHTED SUM OF SQUARED DEVIATIONS                        SETUP
C  [ALSO WEIGHTED BY NUMBER-JJ IF CNTROL(10)=3]                       SETUP
        SUMSQ=SUMSQ+(DELY**2)/(FLOAT(NUMBER-JJ)*ZERO)                 SETUP
                                                                      SETUP
C.. IF CNTROL(10)<0, DON'T CHANGE A- & B-ARRAYS                       SETUP
        IF(CNTROL(10).LE.-1)GOTO 15                                   SETUP
C                              ; NOTE: NEED TO COMPLETE THE DO 15 LOOP SETUP
                                                                      SETUP
        DO 10 K=1,JJ                                                  SETUP
                                                                      SETUP
C       WRITE(2,*)'K=',K                                              SETUP
                                                                      SETUP
        B(K,4)=W*DERIV(K,N,B,Z,BDIM,MDIM,NDIM)                        SETUP
        B(K,3)=B(K,3)+B(K,4)*DELY                                     SETUP
   10   CONTINUE                                                      SETUP
                                                                      SETUP
C.. UP-DATE ON-DIAGONAL AND UPPER-TRIANGLE TERMS OF A-MATRIX          SETUP
        DO 14 J=1,JJ                                                  SETUP
        DO 14 K=J,JJ                                                  SETUP
                                                                      SETUP
C         H=AMAX1(.001*ABS(B(K,1)),1.E-07)                            SETUP
C         DYDJ1=B(J,4)                                                SETUP
C         BHOLD=B(K,1)                                                SETUP
C         B(K,1)=B(K,1)+H                                             SETUP
C         DYDJ2=W*DERIV(J,N,B,Z,BDIM,MDIM,NDIM)                       SETUP
C         B(K,1)=BHOLD                                                SETUP
C         DY2DJK=(DYDJ2-DYDJ1)/H                                      SETUP
C                                                                     SETUP
C         TERM2=-DELY*DY2DJK                                          SETUP
C         TERM1=B(J,4)*B(K,4)                                         SETUP
C       WRITE(2,*)'N=',N                                              SETUP
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C       WRITE(2,*)'J,K=',J,K                                                    SETUP
C         PRINT *,'TERM1,TERM2=',TERM1,TERM2                                    SETUP
C         PRINT *,'DELY,DY2DJK=',DELY,DY2DJK                                    SETUP
                                                                                SETUP
          A(J,K)=A(J,K)+B(J,4)*B(K,4)   ! -  DELY*DY2DJK                        SETUP
                                                                                SETUP
   14     CONTINUE                                                             SETUP
   15     CONTINUE                                                             SETUP
                                                                                SETUP
          DO 444 J=1,BDIM                                                       SETUP
          DO 444 K=1,BDIM                                                       SETUP
C       WRITE(2,*)'J,K=',J,K                                                    SETUP
C       WRITE(2,*)'A(J,K)= ',A(J,K)                                             SETUP
C       WRITE(2,*) B(J,4),B(K,4)=',B(J,4),B(K,4)                                SETUP
 444      CONTINUE                                                             SETUP
          IF(CNTROL(10).LE.-1)GOTO 99                                           SETUP
                                                                                SETUP
C.. FILL-IN LOWER-TRIANGLE OF A-MATRIX WITH IMAGE OF UPPER-TRIANGLE             SETUP
C                       (A-MATRIX IS SYMMETRIC)                                 SETUP
          DO 20 K=2,JJ                                                          SETUP
          L=K-1                                                                 SETUP
          DO 20 J=1,L                                                           SETUP
   20     A(K,J)=A(J,K)                                                        SETUP
                                                                                SETUP
   99     CONTINUE                                                             SETUP
          RETURN                                                                SETUP
          END                                                                   SETUP
      SUBROUTINE MATINV(A,N,B,M,DETERM,IDM)                                     MATINV
                                                                                MATINV
C    MATRIX INVERSION ROUTINE                                                   MATINV
C    CALLED BY GAUSS.FR                                                         MATINV
                                                                                MATINV
C....INPUT:                                                                     MATINV
C       A(K,J) = SUM [ DY/DB(K) * DY/DB(J) ]  ...( FROM SETUP.FR )              MATINV
C       N = ORDER OF A-MATRIX TO INVERT                                         MATINV
C       B(K,1) = SUM [ DY/DB(K) * (YOBS-YCALC) ] ..( = B(K,3) IN GAUSS)         MATINV
C       M = NUMBER OF COLS OF B-MATRIX TO MULTIPLY BY INVERSE OF A-MTX          MATINV
C       IDM = DIMS OF A- & B-MATRICES, MUST BE AT LEAST MAX OF N & M            MATINV
C....OUTPUT:                                                                    MATINV
C       A(  ,  ) = [A]**(-1) = INVERSE OF ORIGINAL A-MATRIX                     MATINV
C       DETERM = DETERMINANT OF A-MATRIX                                        MATINV
C       B(  ,  ) = [A**(-1)] * [B]                                              MATINV
                                                                                MATINV
                                                                                MATINV
          DIMENSION A(IDM,IDM),B(IDM,IDM)                                       MATINV
          DIMENSION IPIVOT(24),INDEX(24,2),PIVOT(24)                            MATINV
          COMMON/DUMMY/IROW,ICOLUM,AMX                                          MATINV
          EQUIVALENCE (IROW,JROW),(ICOLUM,JCOLUM),(AMX,T,SWAP)                  MATINV
                                                                                MATINV
          DETERM=1.0                                                            MATINV
          DO 20 J=1,N                                                           MATINV
   20     IPIVOT(J)=0                                                          MATINV
          DO 550 I=1,N                                                          MATINV
          AMX=0.0                                                               MATINV
          DO 105 J=1,N                                                          MATINV
          IF(IPIVOT(J)-1)60,105,60                                              MATINV
                                                                                MATINV
   60     DO 100 K=1,N                                                         MATINV
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```
      IF(IPIVOT(K)-1)80,100,740                                    MATINV
 80   IF(ABS(AMX)-ABS(A(J,K)))85,100,100                           MATINV
 85   IROW=J                                                       MATINV
      ICOLUM=K                                                     MATINV
      AMX=A(J,K)                                                   MATINV
100   CONTINUE                                                     MATINV
105   CONTINUE                                                     MATINV
      IF(AMX)110,800,110                                           MATINV
110   IPIVOT(ICOLUM)=IPIVOT(ICOLUM)+1                              MATINV
      IF(IROW-ICOLUM)140,260,140                                   MATINV
140   DETERM=-DETERM                                               MATINV
                                                                   MATINV
      DO 200 L=1,N                                                 MATINV
      SWAP=A(IROW,L)                                               MATINV
      A(IROW,L)=A(ICOLUM,L)                                        MATINV
200   A(ICOLUM,L)=SWAP                                             MATINV
      IF(M)260,260,210                                             MATINV
                                                                   MATINV
210   DO 250 L=1,M                                                 MATINV
      SWAP=B(IROW,L)                                               MATINV
      B(IROW,L)=B(ICOLUM,L)                                        MATINV
250   B(ICOLUM,L)=SWAP                                             MATINV
260   INDEX(I,1)=IROW                                              MATINV
      INDEX(I,2)=ICOLUM                                            MATINV
      PIVOT(I)=A(ICOLUM,ICOLUM)                                    MATINV
      DETERM=DETERM*PIVOT(I)                                       MATINV
      A(ICOLUM,ICOLUM)=1.0                                         MATINV
                                                                   MATINV
      DO 350 L=1,N                                                 MATINV
350   A(ICOLUM,L)=A(ICOLUM,L)/PIVOT(I)                             MATINV
      IF(M)380,380,360                                             MATINV
                                                                   MATINV
360   DO 370 L=1,M                                                 MATINV
370   B(ICOLUM,L)=B(ICOLUM,L)/PIVOT(I)                             MATINV
                                                                   MATINV
380   DO 550 L1=1,N                                                MATINV
      IF(L1-ICOLUM)400,550,400                                     MATINV
400   T=A(L1,ICOLUM)                                               MATINV
      A(L1,ICOLUM)=0.0                                             MATINV
                                                                   MATINV
      DO 450 L=1,N                                                 MATINV
450   A(L1,L)=A(L1,L)-A(ICOLUM,L)*T                                MATINV
      IF(M)550,550,460                                             MATINV
                                                                   MATINV
460   DO 500 L=1,M                                                 MATINV
500   B(L1,L)=B(L1,L)-B(ICOLUM,L)*T                                MATINV
550   CONTINUE                                                     MATINV
                                                                   MATINV
      DO 710 I=1,N                                                 MATINV
      L=N+1-I                                                      MATINV
      IF(INDEX(L,1)-INDEX(L,2))630,710,630                         MATINV
630   JROW=INDEX(L,1)                                              MATINV
      JCOLUM=INDEX(L,2)                                            MATINV
                                                                   MATINV
      DO 705 K=1,N                                                 MATINV
      SWAP=A(K,JROW)                                               MATINV
      A(K,JROW)=A(K,JCOLUM)                                        MATINV
      A(K,JCOLUM)=SWAP                                             MATINV
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```
  705     CONTINUE                                                      MATINV
  710     CONTINUE                                                      MATINV
  740     RETURN                                                        MATINV
  800     DETERM=0.                                                     MATINV
          RETURN                                                        MATINV
          END                                                           MATINV
                                                                        MATINV
      SUBROUTINE BTEST(CNTROL,B,BDIM)                                   BTEST
                                                                        BTEST
C     CALLED BY GAUSS.FR                                                BTEST
C                                                                       BTEST
C.. INPUT:                                                            BTEST
C       CNTROL(1) = # PARAMETERS BEING FITTED (ABS VAL)                 BTEST
C       CNTROL(9) = CONVERGENCE CRITERION CONTROL                       BTEST
C                 = 1 OR 2: FCONVG=PCONVG, E.G. 1.E-5                   BTEST
C                 = 3:     FCONVG=BCONVG, E.G. 1.E-2                    BTEST
C       B(J,2)=CURRENT ESTIMATE OF J-TH PARAMETER                       BTEST
C       B(J,3)=INCREMENT TO NEW ESTIMATE OF J-TH PARAMETER              BTEST
C       BDIM=1ST DIMENSION OF B-ARRAY                                   BTEST
C                                                                       BTEST
C.. INTERMEDIATE:                                                     BTEST
C       FCONVG=CONVERGENCE CRITERION                                    BTEST
C                (TEST MADE ON RELATIVE ABSOLUTE DEVIATION)             BTEST
C                                                                       BTEST
C.. OUTPUT:                                                           BTEST
C       CNTROL(21)=1: CAUCHY CONVERGENCE OF PARAMETERS                  BTEST
C                OPTIONAL OUTPUT [IF CNTROL(9).NE.3]                    BTEST
C                B(J,1)=B(J,2)+B(J,3)                                   BTEST
                                                                        BTEST
                                                                        BTEST
        INTEGER CNTROL(25),BDIM                                         BTEST
        REAL B(BDIM,4)                                                  BTEST
        COMMON/CONVG/SCONVG,PCONVG,BCONVG                               BTEST
                                                                        BTEST
        JJ=IABS(CNTROL(1))      ! # PARAMETERS BEING FITTED             BTEST
        FCONVG=PCONVG                                                   BTEST
        IF(CNTROL(9).EQ.3)FCONVG=BCONVG                                 BTEST
                                                                        BTEST
C.. TEST CAUCHY CONVERGENCE OF PARAMETERS                               BTEST
C     WE HAVE CONVERGED WHEN NO PARAMETER IS ESTIMATED TO NEED TO BE    BTEST
C     CHANGED BY MORE THAN A FRACTION FCONVG                            BTEST
        DO 2 J=1,JJ                                                     BTEST
        DENOM=ABS(B(J,2))                                               BTEST
        IF(DENOM.LT.1.0E-8)DENOM=1.0                                    BTEST
        TEST=ABS(B(J,3)/DENOM)                                          BTEST
C.. RETURN IMMEDIATELY [WITHOUT CHANGING CNTROL(21) AND B(J,1)] IF NOT  BTEST
C     CONVERGED                                                         BTEST
        IF(TEST.GT.FCONVG)RETURN                                        BTEST
    2   CONTINUE                                                        BTEST
                                                                        BTEST
        IF(CNTROL(9).EQ.3)GOTO 6                                        BTEST
                                                                        BTEST
C.. IF PARAMETER CONVERGENCE CRITERIA SATISFIED, UP-DATE PARAMETER      BTEST
C     ESTIMATES                                                         BTEST
        DO 3 J=1,JJ                                                     BTEST
    3   B(J,1)=(B(J,2)+B(J,3))                                          BTEST
                                                                        BTEST
C.. SET FLAG TO INDICATE CONVERGENCE                                    BTEST
```

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    6     CNTROL(21)=1                                                    BTEST
          RETURN                                                          BTEST
          END                                                             BTEST
                                                                          BTEST
      SUBROUTINE FINALE(B,Z,MDIM,NDIM,BDIM,A,AV2,SUMSQ)                   FINALE
                                                                          FINALE
C                                                                         FINALE
C.. INPUT:                                                                FINALE
C       B(I)=FITTED VALUE OF I-TH PARAMETER                               FINALE
C       Z(1,N)=OBSERVED VALUE OF Y FOR N-TH DATA POINT                    FINALE
C       Z(MDIM,N)=ERROR IN OBSERVED VALUE OF Y FOR N-TH DATA POINT        FINALE
C       A(I,I)=VARIANCE COEFFICIENT FOR I-TH PARAMETER                    FINALE
C       MDIM=1ST DIMENSION OF Z(  ,  )                                    FINALE
C       NDIM=2ND DIMENSION OF Z(  ,  )                                    FINALE
C       BDIM=DIMENSIONS OF A- AND B-ARRAYS                                FINALE
                                                                          FINALE
C.. INTERMEDIATE:                                                         FINALE
C       SDPRM(I)=STANDARD DEVIATION OF I-TH PARAMETER                     FINALE
C       SS=SUM OF SQUARED DEVIATIONS FOR THE FIT                          FINALE
C       SUMSQ=VARIANCE FOR THE FIT                                        FINALE
C       SDFIT=STANDARD DEVIATION FOR THE FIT                              FINALE
C       AV=AVERAGE DEVIATION                                              FINALE
C       AV1=AVERAGE RELATIVE DEVIATION                                    FINALE
C       YYMAX=MAXIMUM DEVIATION                                           FINALE
C       MARK=POINT WITH YYMAX                                             FINALE
C       ZMAX=MAXIMUM RELATIVE DEVIATION                                   FINALE
C       MARK1=POINT WITH ZMAX                                             FINALE
C       RTMNSQ=ROOT MEAN SQUARE DEVIATION                                 FINALE
                                                                          FINALE
C.. OUTPUT:                                                               FINALE
C       AV2=ERROR=AVERAGE ABSOLUTE RELATIVE DEVIATION                     FINALE
                                                                          FINALE
                                                                          FINALE
        INTEGER CNTROL,BDIM                                               FINALE
        COMMON/CNTROL/CNTROL(25)                                          FINALE
        COMMON/BB/LAB(7,500)                                              FINALE
        DIMENSION Z(MDIM,NDIM),B(BDIM),A(BDIM,BDIM),SDPRM(24)             FINALE
                                                                          FINALE
        JJ=IABS(CNTROL(1))  ! NUMBER PARAMETERS BEING FITTED (ABS VAL)    FINALE
        NUMBER=IABS(CNTROL(3))          ! # DATA POINTS (ABS VAL)         FINALE
        AV=0.                                                             FINALE
        AV1=0.                                                            FINALE
        AV2=0.                                                            FINALE
        YMAX=0.                                                           FINALE
        ZMAX=0.                                                           FINALE
        ZZMAX=0.                                                          FINALE
                                                                          FINALE
C.. TURN OFF A- & B-CHANGING IN SETUP.FR, AND WEIGHT SSQ BY NUMBER-JJ     FINALE
        CNTROL(10)=-2                                                     FINALE
                                                                          FINALE
C.. COMPUTE SUMSQ                                                         FINALE
        CALL SETUP(B,Z,A,SUMSQ,MDIM,NDIM,BDIM)                            FINALE
                                                                          FINALE
        DO 8 I=1,JJ                                                       FINALE
                                                                          FINALE
C.. COMPUTE STANDARD DEVIATION FOR I-TH PARAMETER                         FINALE
    8   SDPRM(I)=SQRT(A(I,I)*SUMSQ)                                       FINALE
                                                                          FINALE
```

```
C.. COMPUTE SUM OF SQUARED DEVIATIONS FOR THIS FIT                      FINALE
      SS=SUMSQ*FLOAT(NUMBER-JJ)                                        FINALE
                                                                       FINALE
C.. COMPUTE STANDARD DEVIATION FOR THIS FIT                            FINALE
      SDFIT=SQRT(SUMSQ)                                                FINALE
      WRITE(2,1)CNTROL(20),(B(J),J=1,JJ)                               FINALE
D     WRITE(6,1)CNTROL(20),(B(J),J=1,JJ)                               FINALE
    1 FORMAT(/,5X,'AFTER  ',I3,' ITERATIONS',/,                        FINALE
     +       8X,'THE MINIMIZING VALUES OF THE PARAMETERS ARE:',/,      FINALE
     +       (1X,1P5E15.7))                                            FINALE
      WRITE(2,12)(SDPRM(I),I=1,JJ)                                     FINALE
D     WRITE(6,12)(SDPRM(I),I=1,JJ)                                     FINALE
   12 FORMAT(/,5X,'WITH THE FOLLOWING STD. DEVIATIONS:',/,             FINALE
     +       (1X,1P5E15.7))                                            FINALE
      WRITE(2,13)SS,SUMSQ,SDFIT                                        FINALE
   13 FORMAT(//,'  THE SUM OF SQUARES,VARIANCE AND SAMPLE STD. DEV',   FINALE
     +       'IATION FOR THIS FIT ARE',1P3E16.5)                       FINALE
                                                                       FINALE
C.. STD DEV OF 1ST PARM                                                FINALE
C.. IS PRINTING OF POINT-BY-POINT COMPARISONS WANTED ?                 FINALE
      IF(CNTROL(7).LT.16)GOTO 90                                       FINALE
                                                                       FINALE
C.. PRINTING OF POINT-BY-POINT COMPARISON WANTED, SO DO IT             FINALE
      WRITE(2,2)                                                       FINALE
    2 FORMAT(//,'************************************************',FINALE
     +      '*************************  ',/)                           FINALE
      WRITE(2,3)                                                       FINALE
    3 FORMAT(//,'NUMBER   LABEL                  Y OBSERVED',         FINALE
     +          '     Y CALCULATED',                                    FINALE
     +       '        OBS-CALC        (OBS-CALC)/OBS   ',/)           FINALE
   90 DO 10 N=1,NUMBER                                                 FINALE
                                                                       FINALE
C.. COMPUTED VALUE OF Y FOR N-THE DATA POINT                           FINALE
      YC=YCOMP(N,B,Z,MDIM,NDIM,BDIM)                                   FINALE
                                                                       FINALE
C.. DEVIATION (OBS-CALC)                                               FINALE
      DELY=Z(1,N)-YC                                                   FINALE
                                                                       FINALE
C.. RELATIVE DEVIATION (RATIO TO OBSERVED VALUE)                       FINALE
      IF(Z(1,N).NE.0.)RATIO=DELY/Z(1,N)                                FINALE
      IF(Z(1,N).EQ.0.)RATIO=1.0E30                                     FINALE
                                                                       FINALE
C.. ABSOLUTE RELATIVE DEVIATION                                        FINALE
      ABSRAT=ABS(RATIO)                                                FINALE
      AV=AV+DELY                                                       FINALE
      AV1=AV1+RATIO                                                    FINALE
      AV2=AV2+ABSRAT                                                   FINALE
      IF(CNTROL(7).GE.16)WRITE(2,5)N,LAB(5,N),LAB(6,N),LAB(7,N),       FINALE
     +                   LAB(1,N),LAB(2,N),Z(1,N),YC,DELY,RATIO        FINALE
    5 FORMAT(I5,3X,5A2,1PE23.5,E17.5,2E19.5)                           FINALE
      ABSVAL=ABS(DELY)                                                 FINALE
                                                                       FINALE
C.. FIND LARGEST ABS DEV                                               FINALE
      IF(YMAX.GT.ABSVAL)GOTO 7                                         FINALE
      YMAX=ABSVAL                                                      FINALE
      YYMAX=DELY                                                       FINALE
      MARK=N                                                           FINALE
                                                                       FINALE
```

```
C.. FIND LARGEST ABS REL DEV                                          FINALE
    7     IF(ZMAX.GT.ABSRAT)GOTO 10                                   FINALE
          ZMAX=ABSRAT                                                 FINALE
          ZZMAX=RATIO                                                 FINALE
          MARK1=N                                                     FINALE
                                                                      FINALE
   10     CONTINUE                                                    FINALE
          D=NUMBER                                                    FINALE
          AV=AV/D                                                     FINALE
          AV1=AV1/D                                                   FINALE
          AV2=AV2/D                                                   FINALE
          RTMNSQ=SQRT(SUMSQ)                                          FINALE
C          WRITE(6,11)AV,AV1,AV2,YYMAX,MARK,ZMAX,MARK1,RTMNSQ         FINALE
          WRITE(2,11)AV,AV1,AV2,YYMAX,MARK,ZMAX,MARK1,RTMNSQ          FINALE
   11     FORMAT(//,                                                  FINALE
     +          '  AVERAGE DEVIATION            ',1PE14.5,/,         FINALE
     +          '        AVERAGE REL DEV        ',E14.5,/,           FINALE
     +          '        AVE ABS REL DEV        ',E14.5,/,           FINALE
     +          '   MAXIMUM DEVIATION           ',E14.5,6X,          FINALE
     +          ' AT POINT ',I4,/,                                    FINALE
     +          '   MAXIMUM REL DEV             ',E14.5,6X,          FINALE
     +          ' AT POINT ',I4,/,                                    FINALE
     +          '   ROOT MEAN SQUARE DEVIATION '  E14.5)             FINALE
                                                                      FINALE
          RETURN                                                      FINALE
          END                                                         FINALE
                                                                      FINALE
      SUBROUTINE PRINDA(CNTROL,Z,MDIM,NDIM)                           PRINDA
                                                                      PRINDA
C     CALLED BY FITSALL.FR                                            PRINDA
                                                                      PRINDA
          INTEGER CNTROL(25)                                          PRINDA
          REAL Z(MDIM,NDIM)                                           PRINDA
                                                                      PRINDA
          N=IABS(CNTROL(3))                                           PRINDA
          NVARS=CNTROL(5)                                             PRINDA
          MN=MINO(NVARS,10)                                           PRINDA
                                                                      PRINDA
          WRITE(2,5)                                                  PRINDA
    5     FORMAT(' INPUT DATA',/,'    I         DV          IV # 1',  PRINDA
     +           '     ......')                                       PRINDA
          DO 20 I=1,N                                                 PRINDA
          WRITE(2,10)I,(Z(J,I),J=1,MN)                                PRINDA
   10     FORMAT(1X,I4,5X,1P10E11.3)                                  PRINDA
          IF(NVARS.GE.11)WRITE(2,15)(Z(J,I),J=11,NVARS)               PRINDA
   15     FORMAT(10X,1P10E11.3)                                       PRINDA
   20     CONTINUE                                                    PRINDA
                                                                      PRINDA
          RETURN                                                      PRINDA
          END                                                         PRINDA
      SUBROUTINE DMPMAT(CNTROL,BDIM,A,B)                              DMPMAT
                                                                      DMPMAT
C     CALLED BY GAUSS.FR                                              DMPMAT
                                                                      DMPMAT
                                                                      DMPMAT
          INTEGER CNTROL(25),BDIM                                     DMPMAT
          DIMENSION A(BDIM,BDIM),B(BDIM)                              DMPMAT
                                                                      DMPMAT
```

```
                                                                      DMPMAT
      WRITE(2,5)                                                      DMPMAT
    5 FORMAT(///'    I    B(I,3)          A(I,1)     A(I,2)    .....')DMPMAT
                                                                      DMPMAT
      JJ=IABS(CNTROL(1))                                              DMPMAT
      MBD=MINO(JJ,10)                                                 DMPMAT
                                                                      DMPMAT
      DO 20 I=1,JJ                                                    DMPMAT
      WRITE(2,10)I,B(I),(A(I,J),J=1,MBD)                              DMPMAT
   10 FORMAT(1HO,I4,2X,1PE10.3,5X,10E11.3)                            DMPMAT
      IF(JJ.GE.11)WRITE(2,15)(A(I,J),J=11,JJ)                         DMPMAT
   15 FORMAT(22X,1P10E11.3)                                           DMPMAT
   20 CONTINUE                                                        DMPMAT
                                                                      DMPMAT
      RETURN                                                          DMPMAT
      END                                                             DMPMAT
     FUNCTION YCOMP(N,B,Z,MDIM,NDIM,BDIM)                             YCOMP
                                                                      YCOMP
                                                                      YCOMP
C.. INPUT:                                                            YCOMP
C       N=DATA POINT INDEX                                            YCOMP
C       B(J)=VALUE OF J-TH PARAMETER                                  YCOMP
C       BDIM=DIMENSION OF B-ARRAY                                     YCOMP
C       MDIM=1ST DIMENSION OF Z-ARRAY                                 YCOMP
C       NDIM=2ND DIMENSION OF Z-ARRAY                                 YCOMP
C       CNTROL(1)= # PARAMETERS BEING FITTED                          YCOMP
C       CNTROL(2)= TOTAL # PARAMETERS                                 YCOMP
C       CNTROL(3)=#DATA POINTS (ABS VAL)                              YCOMP
C       CNTROL(5)=TOTAL NUMBER OF VARIABLES                           YCOMP
C       CNTROL(19)=Y INDEX                                            YCOMP
C       CNTROL(21)=TERMINATION CODE                                   YCOMP
C       CNTROL(22)=COMPUTATION CONTROL FOR YCOMP                      YCOMP
C                 = 0: YCOMP=COMPUTED VALUE OF Y FOR N-TH DATA POINT  YCOMP
C                 > 0: Z(   ,   ) = OBSERVED VALUES FOR N-TH DATA POINT YCOMP
C                                                                     YCOMP
C                                                                     YCOMP
C    INPUT FROM BLANK COMMON:                                         YCOMP
C       X(K,I) = OBSERVED VALUE OF K-TH INDEPENDENT VARIABLE FOR I-TH YCOMP
C                                                                     YCOMP
C       Y(L,I) = OBSERVED VALUE OF L-TH DEPENDENT VARIABLE FOR I-TH   YCOMP
C                                                                     YCOMP
C       E(L,I) = ERROR IN OBSERVED VALUE OF L-TH DEPENDENT VARIABLE   YCOMP
C                                                                     YCOMP
C                                                                     YCOMP
C.. OUTPUT:                                                           YCOMP
C       YCOMP=COMPUTED VALUE OF Y                                     YCOMP
C       Z(1,I)=OBSERVED VALUE OF DEPENDENT VARIABLE Y FOR I-TH DATA PT YCOMP
C       Z(2,I)=OBSERVED VALUE OF 1-ST INDEPENDENT VARIABLE FOR I-TH   YCOMP
C                                                                     YCOMP
C       Z(3,I)=OBSERVED VALUE OF 2-ND INDEPENDENT VARIABLE FOR I-THE  YCOMP
C                                                                     YCOMP
C       Z(4,I)=ERROR IN OBSERVED VALUE OF Y FOR I-TH DATA POINT       YCOMP
C       CNTROL(1)=                                                    YCOMP
                                                                      YCOMP
                                                                      YCOMP
       PARAMETER NDTS=1250                                            YCOMP
       INTEGER CNTROL,BDIM                                            YCOMP
       COMMON/CNTROL/CNTROL(25)                                       YCOMP
```

```
      COMMON X(6,NDTS),Y(1,NDTS),E(1,NDTS)                              YCOMP
      DIMENSION B(BDIM),Z(MDIM,NDIM)                                    YCOMP
                                                                        YCOMP
C.. SPECIAL CASES:                                                      YCOMP
C     1-N: ORDINARY                                                     YCOMP
C     NDIM+1: PARAMETER CHANGE OPTION FROM GAUSS.FR                     YCOMP
C     67: FROM DERIV.FR                                                 YCOMP
C     68: FROM SETUP.FR (1ST DATA POINT)                                YCOMP
C     69: FROM GAUSS.FR (AFTER INCREASING FAC)                          YCOMP
C     70: FROM GAUSS.FR (WHEN PRINTING NORMAL EQNS AFTER MATINV)        YCOMP
                                                                        YCOMP
C      PRINT *,'YCOMP: N,NDIM=',N,NDIM                                  YCOMP
      IF(N.NE.NDIM+1)GOTO 9                                             YCOMP
C      PRINT *,'YCOMP(NDIM+1,'                                          YCOMP
                                                                        YCOMP
C.. SPECIAL CASE [IF N=NDIM+1], ADJUST NUMBER OF PARAMETERS             YCOMP
      ISTORE=CNTROL(1)       ! # PARAMETERS BEING FITTED                YCOMP
                                                                        YCOMP
      IF(CNTROL(21).EQ.0)GOTO 1111                                      YCOMP
C.. NOTE: WORDING OF FOLLOWING STATEMENT ALTERED **********             YCOMP
      IF(CNTROL(1).NE.IABS(CNTROL(2)))GOTO 1108                         YCOMP
      CNTROL(1)=IABS(CNTROL(2))-1                                       YCOMP
      GOTO 1110                                                         YCOMP
 1108 CNTROL(1)=IABS(CNTROL(2))                                         YCOMP
 1110 YCOMP=ISTORE                                                      YCOMP
      RETURN                                                            YCOMP
                                                                        YCOMP
 1111 CNTROL(1)=IABS(CNTROL(2))                                         YCOMP
      GOTO 1110                                                         YCOMP
                                                                        YCOMP
    9 NVARS=CNTROL(5)                                                   YCOMP
      NIV=NVARS-1                                                       YCOMP
      IF(CNTROL(22).EQ.0)GOTO 20                                        YCOMP
                                                                        YCOMP
C.. CNTROL(22)=1, INDICATING INITIAL ENTRY, SO LOAD Z(   ,   ) WITH     YCOMP
C                OBSERVED VALUES                                        YCOMP
      NPTS=IABS(CNTROL(3))   ! # DATA POINTS                            YCOMP
                                                                        YCOMP
      IDV=CNTROL(19)                                                    YCOMP
      IDV=1                                                             YCOMP
      DO 4 I=1,NPTS                                                     YCOMP
      J=1                                                               YCOMP
      Z(1,I)=Y(IDV,I)                ! OBSERVED DV                      YCOMP
C.. IF MDIM GIVES ENOUGH ROOM, LOAD ERROR FOR I-TH DATA POINT           YCOMP
      IF(MDIM.GT.CNTROL(5)) Z(MDIM,I)=E(IDV,I) ! ERR IN OBS DV          YCOMP
      DO 3 K=1,NIV                                                      YCOMP
      J=J+1                                                             YCOMP
      Z(J,I)=X(K,I)                  ! OBSERVED K-TH IV                 YCOMP
   3  CONTINUE                                                          YCOMP
   4  CONTINUE                                                          YCOMP
                                                                        YCOMP
      RETURN                                                            YCOMP
                                                                        YCOMP
C.. CNTROL(22)=0, INDICATING SUBSEQUENT ENTRY, SO COMPUTE VALUE OF Y    YCOMP
  20  NB=IABS(CNTROL(2))          ! TOTAL NUMBER OF PARAMETERS          YCOMP
C      TYPE *,'NB=',NB                                                  YCOMP
      YCOMP=YO(Z(2,N),NIV,B,NB,CNTROL(19))                              YCOMP
C      TYPE *,'YCOMP=',YCOMP                                            YCOMP
```

```
      RETURN                                                            YCOMP
      END                                                               YCOMP
                                                                        YCOMP
      FUNCTION DERIV(K,N,B,Z,BDIM,MDIM,NDIM)                            DERIV
                                                                        DERIV
C.. INPUT:                                                              DERIV
C       K=PARAMETER INDEX                                               DERIV
C       N=DATA POINT INDEX                                              DERIV
C       B(K)=VALUE OF K-TH PARAMETER                                    DERIV
C                                                                       DERIV
C.. OUTPUT:                                                             DERIV
C       DERIV=PARTIAL DERIVATIVE OF Y WITH RESPECT TO K-TH PARAMETER    DERIV
C             AT PARAMETER VALUE B(K) AND IV VALUES OF DATA POINT N     DERIV
C                                                                       DERIV
                                                                        DERIV
      INTEGER BDIM,CNTROL                                               DERIV
      DIMENSION B(BDIM),Z(MDIM,NDIM)                                    DERIV
      COMMON/CNTROL/CNTROL(25)                                          DERIV
                                                                        DERIV
C      PRINT *,'N=',N                                                   DERIV
C      PRINT *,'MDIM,NDIM=',MDIM,NDIM                                   DERIV
                                                                        DERIV
C.. IS ANALTIC DERIVATIVE PROVIDED ?                                    DERIV
      IF(CNTROL(15).EQ.1)GOTO 10                                        DERIV
                                                                        DERIV
C.. HOLD TERMINATION CODE                                               DERIV
      IHOLD=CNTROL(21)                                                  DERIV
C.. TEMPORARILY SET TERMINATION CODE TO 67 (IN CASE YCOMP.FR NEEDS      DERIV
C          TO KNOW THAT THE CALL IS FROM DERIV.FOR                      DERIV
      CNTROL(21)=67                                                     DERIV
      J=K                                                               DERIV
      H=AMAX1(.0001*ABS(B(J)),1.0E-08)                                  DERIV
C.. HOLD B(J)                                                           DERIV
      REMARK=B(J)                                                       DERIV
C.. SHIFT +                                                             DERIV
      B(J)=REMARK+H                                                     DERIV
      Y2=YCOMP(N,B,Z,MDIM,NDIM,BDIM)                                    DERIV
C.. SHIFT -                                                             DERIV
      B(J)=REMARK-H                                                     DERIV
      Y1=YCOMP(N,B,Z,MDIM,NDIM,BDIM)                                    DERIV
C.. RESTORE B(J)                                                        DERIV
      B(J)=REMARK                                                       DERIV
      DERIV=(Y2-Y1)/(2.0*H)                                             DERIV
C.. RESTORE TERMINATION CODE                                            DERIV
      CNTROL(21)=IHOLD                                                  DERIV
      RETURN                                                            DERIV
                                                                        DERIV
C.. ANALYTIC DERIVATIVE                                                 DERIV
 10   NIV=CNTROL(5)-1                                                   DERIV
      NB=IABS(CNTROL(2))                                                DERIV
C      PRINT *,'Z(2,N)=',Z(2,N)                                         DERIV
      DERIV=DYDB(Z(2,N),NIV,B,NB,K,CNTROL(19))                          DERIV
                                                                        DERIV
C     WRITE(2,*)'Z(2,N),NIV,NB,K,CNTROL(19)=',Z(2,N),NIV,NB,K,          DERIV
C    +                                 CNTROL(19)                     DERIV
C     WRITE(2,*)'(B(I),I=1,4)= ',(B(I),I=1,4)                           DERIV
C     WRITE(2,*)'DERIV= ',DERIV                                         DERIV
                                                                        DERIV
```

```
      RETURN                                                            DERIV
      END                                                               DERIV
                                                                        DERIV
      SUBROUTINE ERPROP(B,M3,A,SUM,NB,NIV,IDV,KNTRL3,                   ERPROP
     +                  IOUTER,IPHASE,NTIMES,IDLIFE)                    ERPROP
                                                                        ERPROP
C INPUTS......                                                          ERPROP
C      B=MAX LIKELIHOOD PARAMETER VALUES                                ERPROP
C      M3= TOTAL # OF PARAMETERS                                        ERPROP
C      A=ERROR MATRIX FOR B                                             ERPROP
C      NB=# OF PARAMETERS WHICH WERE FITTED                             ERPROP
C      XD=DESIGN VALUE FOR INDEPENDENT VARIABLES                        ERPROP
C      NIV=# OF INDEPENDENT VARIABLES                                   ERPROP
C      IDV=FUNCT. FORM OPTION SWITCH                                    ERPROP
C        -NEEDS TO BE UP TO DATE (CONSISTENT WITH NUMERICAL PARTIALS)!! ERPROP
                                                                        ERPROP
C OUTPUTS......                                                         ERPROP
C      D=CORROSION DEPTH AT DESIGN-VALUE TIMES                          ERPROP
C      SIGD=UNCERTAINTY IN D                                            ERPROP
                                                                        ERPROP
      PARAMETER NVMAX=1250                                              ERPROP
      PARAMETER (NSTPS = 13)                                            ERPROP
      DIMENSION B(1),A(NB,NB),PYPB(12)                                  ERPROP
      DIMENSION PENREF(NSTPS)                                           ERPROP
      DIMENSION XD(10)                                                  ERPROP
      INTEGER CNTROL                                                    ERPROP
      COMMON/LABEL/LLAB(2)                                              ERPROP
      COMMON/CNTROL/CNTROL(25)                                          ERPROP
      COMMON/XINSERV/XINSERV(5,11),SIGREF(11)                           ERPROP
      COMMON/XV/XVIR(5,NVMAX),IVIR(NVMAX),LVIR(2,NVMAX),                ERPROP
     +          DS(NVMAX),DDS(NVMAX),YVIR(NVMAX)                        ERPROP
                                                                        ERPROP
                                                                        ERPROP
D     WRITE(6,990)                                                      ERPROP
 990  FORMAT(/,1X,'ENTERED MODULE ERPROP')                              ERPROP
                                                                        ERPROP
      WRITE(2,4)                                                        ERPROP
 4    FORMAT(/,'     TIME          DEPTH       UNCERTAINTY',/,          ERPROP
     +       '      YRS         MICROMS        MICROMS')               ERPROP
                                                                        ERPROP
      WNORM=SUM                                                         ERPROP
      TO=0.                                                             ERPROP
      D=0.                                                              ERPROP
C      JTERMC=0                                                         ERPROP
C      IF(CNTROL(21).EQ.5)JTERMC=1                                      ERPROP
      SS=0.                                                             ERPROP
      DO 11 K=1,NB                                                      ERPROP
 11   PYPB(K)=0.                                                        ERPROP
C.. LOOP THROUGH ALL THE TIME STEPS                                     ERPROP
                                                                        ERPROP
      DO 1 I=1,11                                                       ERPROP
                                                                        ERPROP
      DO 61 MM=1,4                                                      ERPROP
      XD(MM)=XINSERV(MM,I)                                              ERPROP
 61   CONTINUE                                                          ERPROP
                                                                        ERPROP
C.. DT=TIME INCREMENT IN YEARS                                          ERPROP
C.. XD(5)=TOTAL TIME IN HOURS                                           ERPROP
```

```
                                                                      ERPROP
      T=XINSERV(5,I)                                                  ERPROP
      DT=T-TO                                                         ERPROP
      XD(5)=(TO+.5*DT)*365.25*24.                                     ERPROP
                                                                      ERPROP
C.. YO IS IN MICROMETERS PER YEAR                                     ERPROP
C.. DD=PENETRATION IN MICROMETERS                                     ERPROP
                                                                      ERPROP
      DD=DT*YO(XD,NIV,B,NB,IDV)                                       ERPROP
      D=D+DD                                                          ERPROP
                                                                      ERPROP
C.. COMPUTE UNCERTAINTY IN INCREMENT TO PENETRATION DURING            ERPROP
C   TIME INTERVAL DT                                                  ERPROP
      SIGD=0.                                                         ERPROP
      DO 2 K=1,NB                                                     ERPROP
      PYPB(K)=PYPB(K)+DT*DYDB(XD,NIV,B,NB,K,IDV)                      ERPROP
      DO 2 J=1,K                                                      ERPROP
      FF=2.                                                           ERPROP
      IF(J.EQ.K) FF=1.                                                ERPROP
  2   SIGD=SIGD+FF*PYPB(J)*PYPB(K)*A(J,K)*WNORM                       ERPROP
C      SIGD=DT*SQRT(SIGD)                                             ERPROP
                                                                      ERPROP
      IF(SIGD.LT.0.)WRITE(2,*)' **WARNING: SIGD= ',SIGD               ERPROP
      IF(SIGD.LT.0.)WRITE(6,*)' **WARNING: SIGD= ',SIGD               ERPROP
      SIGD=ABS(SIGD)                                                  ERPROP
                                                                      ERPROP
                                                                      ERPROP
      SIGD=SQRT(SIGD)                                                 ERPROP
C      WRITE(2) ' SUM,DT,DIGD=',SUM,DT,SIGD                           ERPROP
      IF(IOUTER.NE.0) GOTO 39                                         ERPROP
      SIGREF(I)=SIGD                                                  ERPROP
      PENREF(I)=D                                                     ERPROP
C      IF(I.EQ.IDLIFE) WRITE(8,3)T,D,SIGD                             ERPROP
D     WRITE(6,3)T,D,SIGD,SIGREF(I)-SIGD                               ERPROP
 39   WRITE(2,3) T,D,SIGD,SIGREF(I)-SIGD                              ERPROP
  3   FORMAT(1X,1PE12.3,1P3E15.6)                                     ERPROP
      TO=T                                                            ERPROP
      IF(I.NE.IDLIFE.OR.IOUTER.EQ.0) GOTO 1                           ERPROP
                                                                      ERPROP
      DS(IOUTER)=-SIGREF(I)+SIGD                                      ERPROP
      J=IVIR(IOUTER)                                                  ERPROP
      DDS(J)=-DS(IOUTER)/SIGREF(I)                                    ERPROP
                                                                      ERPROP
      WRITE(2,816) IVIR(IOUTER),LVIR(1,J),LVIR(2,J),                  ERPROP
     +             DS(IOUTER),DDS(J),CNTROL(21)                       ERPROP
816   FORMAT(9X,I5,'-',2I3,2(4X,1PE15.6),2X,I2)                       ERPROP
  1   CONTINUE                                                        ERPROP
                                                                      ERPROP
      DO 12 K=1,NB                                                    ERPROP
      SIGB=SQRT(A(K,K)*WNORM)                                         ERPROP
C      WRITE(6,1000)K,B(K),SIGB                                       ERPROP
C      WRITE(2,1000) K,B(K),SIGB                                      ERPROP
1000  FORMAT(1X,I3,1P2E12.3'   K,B,SIGB')                             ERPROP
 12   CONTINUE                                                        ERPROP
                                                                      ERPROP
      RETURN                                                          ERPROP
      END                                                             ERPROP
     SUBROUTINE RSORT(A,PTR,J,UT,LT)                                  RSORT
```

```
                                                                      RSORT
C.. SORTS ARRAY A(J) BY MAGNITUDE, SMALLEST FIRST                     RSORT
C.. RECORD ORDER IN POINTER ARRAY PTR                                 RSORT
                                                                      RSORT
      INTEGER PTR                                                     RSORT
      INTEGER UT                                                      RSORT
      DIMENSION A(J),UT(J),LT(J),PTR(J)                               RSORT
      INDEX=1                                                         RSORT
      IEND=J                                                          RSORT
      ISTART=1                                                        RSORT
    5 IF((IEND-ISTART).LE.1)GOTO 10                                   RSORT
      MIDPTR=(IEND+ISTART)/2                                          RSORT
      TEMP=A(MIDPTR)                                                  RSORT
      KTEMP=PTR(MIDPTR)                                               RSORT
      A(MIDPTR)=A(ISTART)                                             RSORT
      PTR(MIDPTR)=PTR(ISTART)                                         RSORT
      IENDT=IEND                                                      RSORT
      K=ISTART                                                        RSORT
   20 K=K+1                                                           RSORT
      IF(K.GT.IENDT)GOTO 30                                           RSORT
      IF(A(K).LE.TEMP)GOTO 20                                         RSORT
      IENDF=IENDT+1                                                   RSORT
   40 IENDF=IENDF-1                                                   RSORT
      IF(IENDF.LT.K)GOTO 50                                           RSORT
      IF(A(IENDF).GE.TEMP)GOTO 40                                     RSORT
      X=A(K)                                                          RSORT
      A(K)=A(IENDF)                                                   RSORT
      A(IENDF)=X                                                      RSORT
      X=PTR(K)                                                        RSORT
      PTR(K)=PTR(IENDF)                                               RSORT
      PTR(IENDF)=X                                                    RSORT
      IENDT=IENDF-1                                                   RSORT
      GOTO 20                                                         RSORT
   50 IENDT=K-1                                                       RSORT
   30 A(ISTART)=A(IENDT)                                              RSORT
      A(IENDT)=TEMP                                                   RSORT
      PTR(ISTART)=PTR(IENDT)                                          RSORT
      PTR(IENDT)=KTEMP                                                RSORT
      IF((IENDT+IENDT).LE.(IEND+ISTART))GOTO 60                       RSORT
      LT(INDEX)=ISTART                                                RSORT
      UT(INDEX)=IENDT-1                                               RSORT
      ISTART=IENDT+1                                                  RSORT
      GOTO 70                                                         RSORT
   60 LT(INDEX)=IENDT+1                                               RSORT
      UT(INDEX)=IEND                                                  RSORT
      IEND=IENDT-1                                                    RSORT
   70 INDEX=INDEX+1                                                   RSORT
      GOTO 5                                                          RSORT
   10 IF(ISTART.GE.IEND)GOTO 90                                       RSORT
      IF(A(ISTART).LE.A(IEND))GOTO 90                                 RSORT
      X=A(ISTART)                                                     RSORT
      A(ISTART)=A(IEND)                                               RSORT
      A(IEND)=X                                                       RSORT
      X=PTR(ISTART)                                                   RSORT
      PTR(ISTART)=PTR(IEND)                                           RSORT
      PTR(IEND)=X                                                     RSORT
   90 INDEX=INDEX-1                                                   RSORT
      IF(INDEX.LE.0)RETURN                                            RSORT
```

```
      ISTART=LT(INDEX)                                                  RSORT
      IEND=UT(INDEX)                                                    RSORT
      GOTO 5                                                            RSORT
      END                                                               RSORT
      FUNCTION YO(X,NIV,B,NPARAM,IDV)                                   YO
                                                                        YO
      DIMENSION X(1), B(1)                                              YO
                                                                        YO
C       WRITE(2,*)'NPARAM= ',NPARAM                                     YO
C       WRITE(2,*)'(X(I),I=1,5)= ',(X(I),I=1,5)                         YO
C       WRITE(2,*)'(B(I),I=1,4)= ',(B(I),I=1,4)                         YO
                                                                        YO
C.. BRANCH ACCORDING TO NUMBER OF PARAMETERS BEING FITTED               YO
      GOTO (1,2,3,4,5,6),NPARAM                                         YO
                                                                        YO
C.. FIT USING B(1) ONLY: OVERALL LEVEL                                  YO
   1  P=B(1)/(1450.0+SQRT(X(5)))                                       YO
   2  Q=(1.E-6*(X(2)*10000./32.+X(4)/4./18.)+18100.0*X(3)-5793.)/      YO
     +           (X(1)+273.)                                          YO
      IF(NPARAM.EQ.1) GOTO 100                                          YO
                                                                        YO
C.. ADD B(2):  TIME                                                     YO
      GOTO 10                                                           YO
                                                                        YO
C.. ADD B(3):  MAGNESIUM                                                YO
   3  Q=(1.E-6*(X(2)*10000./32.+X(4)/4./18.)+B(3)*X(3)-5793.)/         YO
     +   (X(1)+273.)                                                   YO
      GOTO 10                                                           YO
                                                                        YO
C.. ADD B(4):  OXYGEN                                                   YO
   4  Q=(B(4)*(X(2)*10000./32.+X(4)/4./18.)+B(3)*X(3)-5793.)/          YO
     +   (X(1)+273.)                                                   YO
      GOTO 10                                                           YO
                                                                        YO
C.. ADD B(5):  O2 & H2O SEPARATELY                                      YO
   5  Q=(B(5)*X(2)+B(3)*X(3)+B(4)*X(4)-5793.)/(X(1)+273.)              YO
      GOTO 10                                                           YO
                                                                        YO
C.. ADD B(6):  TEMPERATURE                                              YO
   6  Q=(B(5)*X(2)+B(3)*X(3)+B(4)*X(4)-B(6))/(X(1)+273.)               YO
                                                                        YO
  10  P=B(1)/(B(2)+SQRT(X(5)))                                          YO
                                                                        YO
 100  IF(IDV.NE.2)YO=P*EXP(Q)                                           YO
      IF(IDV.EQ.2)YO=ALOG(P)+Q                                          YO
                                                                        YO
C      WRITE(2,*)'P,Q,YO= ',P,Q,YO                                      YO
                                                                        YO
      RETURN                                                            YO
      END                                                               YO
                                                                        YO
      FUNCTION DYDB(X,NIV,B,NB,K,IDV)                                   DYDB
                                                                        DYDB
                                                                        DYDB
        DIMENSION X(NIV),B(NB)                                          DYDB
                                                                        DYDB
        EE=1.                                                           DYDB
        IF(IDV.NE.2)EE=YO(X,NIV,B,NB,IDV)                               DYDB
```

```
                                                                      DYDB
      GOTO(1,2,3,4,5,6),K                                             DYDB
                                                                      DYDB
1     DYDB=EE/B(1)                                                    DYDB
      RETURN                                                          DYDB
                                                                      DYDB
2     DYDB=-EE/(B(2)*SQRT(X(5)))                                      DYDB
      RETURN                                                          DYDB
                                                                      DYDB
3     DYDB=EE*X(3)/(X(1)+273.)                                        DYDB
      RETURN                                                          DYDB
                                                                      DYDB
4     IF(NB.EQ.4)DYDB=EE*(X(2)*10000./32.+X(4)/4./18.)/(X(1)+273.)    DYDB
      IF(NB.GE.5)DYDB=EE*X(4)/(X(1)+273.)                             DYDB
      RETURN                                                          DYDB
                                                                      DYDB
5     DYDB=EE*X(2)/(X(1)+273.)                                        DYDB
      RETURN                                                          DYDB
                                                                      DYDB
6     DYDB=-EE/(X(1)+273.)                                            DYDB
      RETURN                                                          DYDB
                                                                      DYDB
      END                                                             DYDB
```

C.2.1 Annotated Sample Output from UNODEX

```
UNODEX  V1.0:                    WASTE CONTAINER PENETRATION UNCERTAINTY                    19-JAN-87  23:34:48
                                      ***5 REF MATRIX, 300 YEAR
                                        20,000 HR MAX TIME

                                    EVALUATION OF ESS   201

**********************************************
* BEGIN INPUT PROBLEM AND JOB CONTROL DATA *
**********************************************
C. Edited echo of input data follows.
C.
C. JADD is the value of virtual data points which have been permanently shifted into the ESS.
C. At this level in the program the value is zero and initial parameter fitting follows, along with
C. pointwise sequential evaluation of the ESS virtual data.
 * * * * * * * * * * * * * * * * * * * * *
         JADD =          0
 * * * * * * * * * * * * * * * * * * * * *

 MINIMUM CORE DIMENSION =     1312
 NONLINEAR REGRESSION CONTROLS ARE:
        1    2    3    4    5    6    7    8    9   10   11   12   13   14   15   16   17   18   19
        3    3 -187    4    6   70   31    6    1    4    0    1    0    0    1    1    1    1    1
 NUMBER OF PARAMETERS                          3
 NUMBER OF DATA POINTS                       182
 NUMBER OF VARIABLES                           6
 LIMIT ON NUMBER OF ITERATIONS                70

 CONVERGENCE CRITERIA:       SCONVG =  5.000E-07       PCONVG =  1.000E-05       BCONVG =  1.000E-02

 THE FOLLOWING INFORMATION IS TO BE PRINTED OUT:
C. All the print options are invoked on this run, an abbreviated sample follows.

 INPUT DATA    SUMSQ AND PARAMETER VALUES    NORMAL EQ MATRICES    RESTRAINED CHANGE MECHANISM    POINT BY POINT COMPARISON
     YES                   YES                    YES                    YES                            YES

 CNTROL(8) =  6 SO MINIMIZE LEAST SQUARES                    WEIGHTED BY '1/Z(C5,N) )
 CNTROL(10) NONZERO, PARAMETERS CAN CHANGE BY AT MOST  40 PERCENT
 STARTING GUESSES FOR THE PARAMETERS B(J)
       J :        1             2             3
      B(J):   2.3500E+11    1.4500E+03    1.6100E+04

 NONLINEAR REGRESSION ARRAY DIMENSIONS ARE:
      ERROR MATRIX:          Z( 7,182)
      PARAMETERS:            B( 4)



**********************************************
* BEGIN INTERMEDIATE NORMAL EQUATION MATRICIES*
**********************************************
C. Input data echo, one example follows, this option will be omitted subsequently, and replaced
C. with "INPUT DATA"
C.
 INPUT DATA
    I        DV          IV # 1      ......
    1      2.082E+01   1.500E+02   5.000E-02   1.000E-04   7.600E+01   6.980E+02
    2      1.111E+01   1.500E+02   5.000E-02   1.000E-04   7.600E+01   5.835E+03
    3      1.285E+01   1.500E+02   5.000E-02   1.000E-04   7.600E+01   5.835E+03
```

4	1.036E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	5.635E+03
5	1.215E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	5.635E+03
6	1.332E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	5.635E+03
7	1.525E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	2.897E+03
8	1.681E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	5.321E+03
9	1.823E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	5.321E+03
10	1.671E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	5.321E+03
11	1.894E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	6.980E+02
12	1.845E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	5.321E+03
13	1.309E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	5.321E+03
14	1.302E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	2.897E+03
15	1.888E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	5.321E+03
16	2.853E+01	1.500E+02	1.500E+00	1.000E-04	7.600E+01	5.384E+03
17	2.174E+01	1.500E+02	1.500E+00	1.000E-04	7.600E+01	5.384E+03
18	2.760E+01	1.500E+02	1.500E+00	1.000E-04	7.600E+01	2.908E+03
19	2.818E+01	1.500E+02	1.500E+00	1.000E-04	7.600E+01	7.360E+02
20	2.855E+01	1.500E+02	1.500E+00	1.000E-04	7.600E+01	5.384E+03
21	3.034E+01	1.500E+02	1.500E+00	1.000E-04	7.600E+01	5.384E+03
22	2.411E+01	1.500E+02	1.500E+00	1.000E-04	7.600E+01	5.384E+03
23	1.494E+01	1.500E+02	1.500E+00	1.000E-04	7.600E+01	2.908E+03
24	2.129E+01	1.500E+02	1.500E+00	1.000E-04	7.600E+01	5.384E+03
25	2.831E+01	1.500E+02	1.500E+00	1.000E-04	7.600E+01	7.360E+02
26	2.343E+01	1.500E+02	1.500E+00	1.000E-04	7.600E+01	5.384E+03
27	2.178E+01	1.500E+02	1.500E+00	1.000E-04	7.600E+01	5.384E+03
28	2.869E+01	1.500E+02	1.500E+00	1.000E-04	7.600E+01	5.384E+03
29	2.941E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	7.680E+02
30	1.831E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	2.180E+03
31	1.436E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	3.974E+03
32	1.544E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	5.099E+03
33	1.160E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	3.974E+03
34	1.253E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	5.099E+03
35	1.023E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	3.974E+03
36	1.286E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	5.099E+03
37	1.387E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	7.680E+02
38	4.837E+02	1.500E+02	5.000E-02	4.200E-03	5.000E+00	2.178E+03
39	4.293E+02	1.500E+02	5.000E-02	4.200E-03	5.000E+00	2.178E+03
40	4.881E+02	1.500E+02	5.000E-02	4.200E-03	5.000E+00	2.178E+03
41	4.990E+02	1.500E+02	5.000E-02	4.200E-03	5.000E+00	2.178E+03
42	4.898E+02	1.500E+02	5.000E-02	4.200E-03	5.000E+00	2.178E+03
43	4.422E+02	1.500E+02	5.000E-02	4.200E-03	5.000E+00	2.178E+03
44	4.989E+02	1.500E+02	5.000E-02	8.400E-03	1.000E+01	2.178E+03
45	5.656E+02	1.500E+02	5.000E-02	8.100E-03	1.000E+01	2.178E+03
46	5.377E+02	1.500E+02	5.000E-02	8.100E-03	1.000E+01	2.178E+03
47	5.892E+02	1.500E+02	5.000E-02	8.100E-03	1.000E+01	2.178E+03
48	4.828E+02	1.500E+02	5.000E-02	8.100E-03	1.000E+01	2.178E+03
49	5.340E+02	1.500E+02	5.000E-02	8.100E-03	1.000E+01	2.178E+03
50	6.873E+02	1.500E+02	5.000E-02	1.700E-02	2.000E+01	2.178E+03
51	6.463E+02	1.500E+02	5.000E-02	1.700E-02	2.000E+01	2.178E+03
52	6.563E+02	1.500E+02	5.000E-02	1.700E-02	2.000E+01	2.178E+03
53	6.694E+02	1.500E+02	5.000E-02	1.700E-02	2.000E+01	2.178E+03
54	6.605E+02	1.500E+02	5.000E-02	1.700E-02	2.000E+01	2.178E+03
55	6.913E+02	1.500E+02	5.000E-02	1.700E-02	2.000E+01	2.178E+03
56	6.646E+02	1.500E+02	5.000E-02	2.200E-02	2.500E+01	2.178E+03
57	7.392E+02	1.500E+02	5.000E-02	2.200E-02	2.500E+01	2.178E+03
58	6.151E+02	1.500E+02	5.000E-02	2.200E-02	2.500E+01	2.178E+03
59	5.195E+02	1.500E+02	5.000E-02	2.200E-02	2.500E+01	2.178E+03
60	6.267E+02	1.500E+02	5.000E-02	2.200E-02	2.500E+01	2.178E+03
61	6.222E+02	1.500E+02	5.000E-02	2.200E-02	2.500E+01	2.178E+03
62	6.214E+02	1.500E+02	5.000E-02	2.700E-02	3.000E+01	2.178E+03
63	7.474E+02	1.500E+02	5.000E-02	2.700E-02	3.000E+01	2.178E+03
64	5.963E+02	1.500E+02	5.000E-02	2.700E-02	3.000E+01	2.178E+03
65	5.889E+02	1.500E+02	5.000E-02	2.700E-02	3.000E+01	2.178E+03

128	7.933E+02	1.500E+02	5.000E-02	4.680E-02	7.600E+01	1.440E+02
129	5.880E+02	1.500E+02	5.000E-02	4.680E-02	7.600E+01	3.300E+02
130	2.244E+02	1.500E+02	5.000E-02	4.900E-03	7.600E+01	7.510E+02
131	2.459E+02	1.500E+02	5.000E-02	4.900E-03	7.600E+01	7.510E+02
132	5.649E+02	1.500E+02	5.000E-02	4.680E-02	7.600E+01	3.350E+02
133	1.457E+03	1.500E+02	5.000E-02	4.680E-02	7.600E+01	3.350E+02
134	5.409E+02	1.500E+02	5.000E-02	4.680E-02	7.600E+01	3.370E+02
135	1.928E+03	1.500E+02	5.000E-02	4.680E-02	7.600E+01	3.360E+02
136	1.300E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	3.360E+02
137	5.979E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	3.360E+02
138	1.117E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	3.360E+02
139	5.694E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	3.360E+02
140	2.878E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	3.360E+02
141	8.140E+01	1.500E+02	5.000E-02	1.000E-04	7.600E+01	3.360E+02
142	7.320E+00	1.500E+02	5.000E-02	1.000E-04	2.000E+01	2.198E+03
143	1.018E+01	1.500E+02	5.000E-02	1.000E-04	2.000E+01	2.198E+03
144	1.031E+01	1.500E+02	5.000E-02	1.000E-04	2.000E+01	2.198E+03
145	5.350E+01	9.000E+01	5.000E-02	1.340E-02	2.000E+01	2.203E+03
146	5.548E+01	9.000E+01	5.000E-02	1.340E-02	2.000E+01	2.203E+03
147	8.768E+01	9.000E+01	5.000E-02	1.340E-02	2.000E+01	2.203E+03
148	4.344E+01	9.000E+01	5.000E-02	1.340E-02	2.000E+01	2.203E+03
149	4.546E+01	9.000E+01	5.000E-02	1.340E-02	2.000E+01	2.203E+03
150	2.382E+01	9.000E+01	5.000E-02	1.340E-02	2.000E+01	2.203E+03
151	4.891E+02	1.500E+02	5.000E-02	1.340E-02	2.000E+01	2.179E+03
152	5.598E+02	1.500E+02	5.000E-02	1.340E-02	2.000E+01	2.179E+03
153	3.883E+02	1.500E+02	5.000E-02	1.340E-02	2.000E+01	2.179E+03
154	2.475E+01	1.500E+02	5.000E-02	1.000E-04	2.000E+01	2.179E+03
155	2.078E+01	1.500E+02	5.000E-02	1.000E-04	2.000E+01	2.179E+03
156	4.430E+00	1.500E+02	5.000E-02	1.000E-04	2.000E+01	2.179E+03
157	1.769E+01	1.500E+02	5.000E-02	1.000E-04	2.000E+01	2.155E+03
158	2.518E+01	1.500E+02	5.000E-02	1.000E-04	2.000E+01	2.155E+03
159	1.888E+01	1.500E+02	5.000E-02	1.000E-04	2.000E+01	2.155E+03
160	7.830E+00	9.000E+01	5.000E-02	1.000E-04	2.000E+01	2.155E+03
161	8.780E+00	9.000E+01	5.000E-02	1.000E-04	2.000E+01	2.155E+03
162	8.370E+00	9.000E+01	5.000E-02	1.000E-04	2.000E+01	2.155E+03
163	8.330E+00	1.500E+02	5.000E-02	1.000E-04	5.000E+00	2.155E+03
164	8.670E+00	1.500E+02	5.000E-02	1.000E-04	5.000E+00	2.155E+03
165	8.150E+00	1.500E+02	5.000E-02	1.000E-04	5.000E+00	2.155E+03
166	3.090E+00	9.000E+01	5.000E-02	1.000E-04	5.000E+00	2.155E+03
167	3.080E+00	9.000E+01	5.000E-02	1.000E-04	5.000E+00	2.155E+03
168	2.900E+00	9.000E+01	5.000E-02	1.000E-04	5.000E+00	2.155E+03
169	1.078E+02	2.000E+02	5.000E-02	1.000E-04	5.000E+00	2.155E+03
170	8.943E+01	2.000E+02	5.000E-02	1.000E-04	5.000E+00	2.155E+03
171	8.083E+01	2.000E+02	5.000E-02	1.000E-04	5.000E+00	2.155E+03
172	4.220E+02	1.500E+02	5.000E-02	3.400E-03	5.000E+00	2.155E+03
173	3.330E+02	1.500E+02	5.000E-02	3.400E-03	5.000E+00	2.155E+03
174	3.203E+02	1.500E+02	5.000E-02	3.400E-03	5.000E+00	2.155E+03
175	1.183E+01	9.000E+01	5.000E-02	3.400E-03	5.000E+00	2.155E+03
176	1.651E+01	9.000E+01	5.000E-02	3.400E-03	5.000E+00	2.155E+03
177	1.090E+01	9.000E+01	5.000E-02	3.400E-03	5.000E+00	2.155E+03
178	8.817E+02	2.000E+02	5.000E-02	3.400E-03	5.000E+00	2.155E+03
179	8.832E+02	2.000E+02	5.000E-02	3.400E-03	5.000E+00	2.155E+03
180	9.500E+02	2.000E+02	5.000E-02	3.400E-03	5.000E+00	2.155E+03
181	8.259E+02	2.000E+02	5.000E-02	3.400E-03	5.000E+00	2.155E+03
182	8.688E+02	2.000E+02	5.000E-02	3.400E-03	5.000E+00	2.155E+03

C. Now the normal equations follow,
C. See Source Listing for comments defining B(,) and A(,)

	I	B(I,3)	A(I,1)	A(I,2)	.....
0	1	3.581E-11	1.461E-20	-2.306E-12	2.540E-13
0	2	-5.815E-03	-2.306E-12	3.640E-04	-4.018E-05
0	3	9.852E-04	2.540E-13	-4.018E-05	5.867E-06

66	6.158E+02	1.500E+02	5.000E-02	2.700E-02	3.000E+01	2.178E+03
67	8.085E+02	1.500E+02	5.000E-02	2.700E-02	3.000E+01	2.178E+03
68	4.159E+02	1.500E+02	5.000E-02	1.700E-02	2.000E+01	7.031E+03
69	4.079E+02	1.500E+02	5.000E-02	1.700E-02	2.000E+01	7.031E+03
70	4.208E+02	1.500E+02	5.000E-02	1.700E-02	2.000E+01	7.031E+03
71	4.637E+02	1.500E+02	5.000E-02	1.700E-02	2.000E+01	7.031E+03
72	4.052E+02	1.500E+02	5.000E-02	1.700E-02	2.000E+01	7.031E+03
73	4.263E+02	1.500E+02	5.000E-02	1.700E-02	2.000E+01	7.031E+03
74	7.770E+02	1.500E+02	5.000E-02	2.700E-02	3.000E+01	1.659E+03
75	7.933E+02	1.500E+02	5.000E-02	2.700E-02	3.000E+01	1.659E+03
76	6.998E+02	1.500E+02	5.000E-02	2.700E-02	3.000E+01	1.659E+03
77	6.256E+02	1.500E+02	5.000E-02	2.700E-02	3.000E+01	1.659E+03
78	5.580E+02	1.500E+02	5.000E-02	2.700E-02	3.000E+01	1.659E+03
79	6.922E+02	1.500E+02	5.000E-02	2.700E-02	3.000E+01	1.659E+03
80	5.416E+02	1.500E+02	5.000E-02	1.700E-02	2.000E+01	7.670E+02
81	6.683E+02	1.500E+02	5.000E-02	1.700E-02	2.000E+01	7.670E+02
82	5.882E+02	1.500E+02	5.000E-02	1.700E-02	2.000E+01	7.670E+02
83	7.216E+02	1.500E+02	5.000E-02	1.700E-02	2.000E+01	7.670E+02
84	6.540E+02	1.500E+02	5.000E-02	1.700E-02	2.000E+01	7.670E+02
85	5.378E+02	1.500E+02	5.000E-02	1.700E-02	2.000E+01	7.670E+02
86	6.212E+02	1.500E+02	5.000E-02	2.700E-02	3.000E+01	7.670E+02
87	6.536E+02	1.500E+02	5.000E-02	2.700E-02	3.000E+01	7.670E+02
88	5.282E+02	1.500E+02	5.000E-02	2.700E-02	3.000E+01	7.670E+02
89	6.079E+02	1.500E+02	5.000E-02	2.700E-02	3.000E+01	7.670E+02
90	5.942E+02	1.500E+02	5.000E-02	2.700E-02	3.000E+01	7.670E+02
91	5.881E+02	1.500E+02	5.000E-02	2.700E-02	3.000E+01	7.670E+02
92	1.207E+01	1.500E+02	5.000E-02	4.000E-04	2.000E+01	7.590E+02
93	1.256E+01	1.500E+02	5.000E-02	4.000E-04	2.000E+01	7.590E+02
94	1.080E+01	1.500E+02	5.000E-02	4.000E-04	2.000E+01	7.590E+02
95	8.355E+00	1.500E+02	5.000E-02	4.000E-04	2.000E+01	7.590E+02
96	7.276E+02	1.500E+02	5.000E-02	1.700E-02	2.000E+01	7.600E+02
97	5.538E+02	1.500E+02	5.000E-02	1.700E-02	2.000E+01	7.600E+02
98	4.911E+02	1.500E+02	5.000E-02	1.700E-02	2.000E+01	7.600E+02
99	5.383E+02	1.500E+02	5.000E-02	1.700E-02	2.000E+01	7.600E+02
100	8.116E+02	1.500E+02	5.000E-02	4.680E-02	7.600E+01	7.620E+02
101	8.460E+02	1.500E+02	5.000E-02	4.680E-02	7.600E+01	7.620E+02
102	7.978E+02	1.500E+02	5.000E-02	4.680E-02	7.600E+01	2.181E+03
103	7.578E+02	1.500E+02	5.000E-02	4.680E-02	7.600E+01	2.181E+03
104	1.157E+03	1.500E+02	5.000E-02	4.690E-02	7.600E+01	7.230E+02
105	1.133E+03	1.500E+02	5.000E-02	4.690E-02	7.600E+01	7.230E+02
106	1.048E+03	1.500E+02	5.000E-02	4.690E-02	7.600E+01	2.540E+03
107	1.042E+03	1.500E+02	5.000E-02	4.690E-02	7.600E+01	2.540E+03
108	9.373E+02	1.500E+02	5.000E-02	4.690E-02	7.600E+01	4.294E+03
109	9.479E+02	1.500E+02	5.000E-02	4.690E-02	7.600E+01	4.294E+03
110	4.525E+01	9.000E+01	5.000E-02	4.650E-02	7.600E+01	7.450E+02
111	6.824E+01	9.000E+01	5.000E-02	4.650E-02	7.600E+01	7.450E+02
112	5.725E+01	9.000E+01	5.000E-02	4.650E-02	7.600E+01	2.163E+03
113	3.906E+01	9.000E+01	5.000E-02	4.650E-02	7.600E+01	2.163E+03
114	5.626E+01	9.000E+01	5.000E-02	4.650E-02	7.600E+01	4.424E+03
115	5.639E+01	9.000E+01	5.000E-02	4.650E-02	7.600E+01	4.424E+03
116	6.797E+02	1.500E+02	5.000E-02	3.530E-02	5.300E+01	7.200E+02
117	6.955E+02	1.500E+02	5.000E-02	3.530E-02	5.300E+01	7.200E+02
118	9.421E+02	1.500E+02	5.000E-02	3.530E-02	5.300E+01	2.124E+03
119	9.165E+02	1.500E+02	5.000E-02	3.530E-02	5.300E+01	2.124E+03
120	2.802E+01	9.000E+01	5.000E-02	3.270E-02	5.300E+01	6.720E+02
121	3.373E+01	9.000E+01	5.000E-02	3.270E-02	5.300E+01	6.720E+02
122	2.955E+01	9.000E+01	5.000E-02	3.270E-02	5.300E+01	2.119E+03
123	2.608E+01	9.000E+01	5.000E-02	3.270E-02	5.300E+01	2.119E+03
124	1.648E+02	1.500E+02	5.000E-02	9.000E-04	7.600E+01	6.770E+02
125	1.521E+02	1.500E+02	5.000E-02	9.000E-04	7.600E+01	6.770E+02
126	4.212E+02	1.500E+02	5.000E-02	1.020E-02	7.600E+01	7.730E+02
127	4.145E+02	1.500E+02	5.000E-02	1.020E-02	7.600E+01	7.730E+02

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CYCLE     SUM OF SQUARES        ********** B(J) PARAMETERS  **********

0 0         2.0872446E+02          2.3500000E+11  1.4500000E+03  1.6100000E+04


     I     B(I,3)          A(I,1)      A(I,2)      .....
0    1   -5.714E+1:       6.347E+23  4.048E+15  2.411E+14
0    2   -3.833E+03       4.048E+15  2.582E+07  1.615E+06
0    3    2.272E+01       2.411E+14  1.615E+06  7.901E+05

 S PARAMETERS

   2.3500E+11 -9.4000E+10 -5.7142E+11 -1.0000E+00
   1.4500E+03 -5.8000E+02 -3.6332E+03 -1.0000E+00
   1.6100E+04  6.4400E+03  2.2718E+01  1.0000E+00

CYCLE     SUM OF SQUARES        ********** B(J) PARAMETERS  **********

0 1         2.0690790E+02          1.4100000E+11  8.7000000E+02  1.6122718E+04

 NO REDUCTION IN SUM OF SQUARES. RESCALE PARAMETERS

 RESTRAINED CHANGE MECHANISM SETAT ( 0.2000E+00+ 0.0000) TIMES THE VALUE OF THE ORIGINAL PARAMETER

CYCLE     SUM OF SQUARES        ********** B(J) PARAMETERS  **********

0 1         2.0672847E+02          1.8800001E+11  1.1600000E+03  1.6111359E+04

 NO REDUCTION IN SUM OF SQUARES. RESCALE PARAMETERS

 RESTRAINED CHANGE MECHANISM SETAT ( 0.1000E+00+ 0.0000) TIMES THE VALUE OF THE ORIGINAL PARAMETER

CYCLE     SUM OF SQUARES        ********** B(J) PARAMETERS  **********

0 1         2.0671628E+02          2.1150001E+11  1.3050000E+03  1.6105880E+04
 NEW SQMIN=    2.067163E+02


     I     B(I,3)          A(I,1)      A(I,2)      .....
0    1    4.921E-11        1.794E-20 -2.824E-12  2.810E-13
0    2   -7.933E-03       -2.824E-12  4.446E-04 -4.434E-05
0    3    1.103E-03        2.810E-13 -4.434E-05  5.844E-06

CYCLE     SUM OF SQUARES        ********** B(J) PARAMETERS  **********

0 1         2.0671628E+02          2.1150001E+11  1.3050000E+03  1.6105880E+04


     I     B(I,3)          A(I,1)      A(I,2)      .....
0    1   -4.388E+11       4.213E+23  2.398E+15  1.982E+14
0    2   -2.804E+03       2.69CE+15  1.726E+07  1.326E+06
0    3    1.522E+01       1.982E+14  1.326E+06  7.950E+05

 S PARAMETERS

   2.1150E+11 -8.4600E+10 -4.3877E+11 -1.0000E+00
   1.3050E+03 -5.2200E+02 -2.7036E+03 -1.0000E+00
   1.6106E+04  6.4423E+03  1.5218E+01  1.0000E+00

CYCLE     SUM OF SQUARES        ********** B(J) PARAMETERS  **********
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 0 2        2.0707491E+02        1.2890000E+11  7.8300000E+02  1.6120897E+04
 NO REDUCTION IN SUM OF SQUARES. RESCALE PARAMETERS
 RESTRAINED CHANGE MECHANISM SETAT ( 0.2000E+00+ 0.0000) TIMES THE VALUE OF THE ORIGINAL PARAMETER
CYCLE    SUM OF SQUARES        ********** B(J) PARAMETERS  **********
 0 2        2.0677219E+02        1.6920001E+11  1.0440000E+03  1.6113288E+04
 NO REDUCTION IN SUM OF SQUARES. RESCALE PARAMETERS
 RESTRAINED CHANGE MECHANISM SETAT ( 0.1000E+00+ 0.0000) TIMES THE VALUE OF THE ORIGINAL PARAMETER
CYCLE    SUM OF SQUARES        ********** B(J) PARAMETERS  **********
 0 2        2.0672910E+02        1.9035000E+11  1.1745000E+03  1.6109484E+04
 NO REDUCTION IN SUM OF SQUARES. RESCALE PARAMETERS
 RESTRAINED CHANGE MECHANISM SETAT ( 0.5000E-01+ 0.0000) TIMES THE VALUE OF THE ORIGINAL PARAMETER
CYCLE    SUM OF SQUARES        ********** B(J) PARAMETERS  **********
 0 2        2.0672008E+02        2.0092500E+11  1.2397500E+03  1.6107582E+04
 NO REDUCTION IN SUM OF SQUARES. RESCALE PARAMETERS
 RESTRAINED CHANGE MECHANISM SETAT ( 0.2500E-01+ 0.0000) TIMES THE VALUE OF THE ORIGINAL PARAMETER
CYCLE    SUM OF SQUARES        ********** B(J) PARAMETERS  **********
 0 2        2.0671765E+02        2.0621251E+11  1.2723750E+03  1.6106631E+04
 NO REDUCTION IN SUM OF SQUARES. RESCALE PARAMETERS
 RESTRAINED CHANGE MECHANISM SETAT ( 0.1250E-01+ 0.0000) TIMES THE VALUE OF THE ORIGINAL PARAMETER
CYCLE    SUM OF SQUARES        ********** B(J) PARAMETERS  **********
 0 2        2.0671690E+02        2.0885625E+11  1.2886875E+03  1.6106155E+04
 NO REDUCTION IN SUM OF SQUARES. RESCALE PARAMETERS
 RESTRAINED CHANGE MECHANISM SETAT ( 0.6250E-02+ 0.0000) TIMES THE VALUE OF THE ORIGINAL PARAMETER
CYCLE    SUM OF SQUARES        ********** B(J) PARAMETERS  **********
 0 2        2.0671671E+02        2.1017813E+11  1.2968438E+03  1.6105917E+04
 NO REDUCTION IN SUM OF SQUARES. RESCALE PARAMETERS
 RESTRAINED CHANGE MECHANISM SETAT ( 0.3125E-02+ 0.0000) TIMES THE VALUE OF THE ORIGINAL PARAMETER
CYCLE    SUM OF SQUARES        ********** B(J) PARAMETERS  **********
 0 2        2.0671648E+02        2.1083908E+11  1.3009219E+03  1.6105799E+04
 NO REDUCTION IN SUM OF SQUARES. RESCALE PARAMETERS
 RESTRAINED CHANGE MECHANISM SETAT ( 0.1563E-02+ 0.0000) TIMES THE VALUE OF THE ORIGINAL PARAMETER
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CYCLE    SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************
0 2        2.0671628E+02         2.1118954E+11  1.3029609E+03  1.6105739E+04
CYCLE    SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************
0 3        2.1690285E+02         4.2299998E+10  2.6100000E+02  1.6120897E+04
 NO REDUCTION IN SUM OF SQUARES. RESCALE PARAMETERS
 RESTRAINED CHANGE MECHANISM SETAT ( 0.2000E+00+ 0.4000) TIMES THE VALUE OF THE ORIGINAL PARAMETER
CYCLE    SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************
0 3        2.0848851E+02         8.4599998E+10  5.2200000E+02  1.6113288E+04
 NO REDUCTION IN SUM OF SQUARES. RESCALE PARAMETERS
 RESTRAINED CHANGE MECHANISM SETAT ( 0.1000E+00+ 0.4000) TIMES THE VALUE OF THE ORIGINAL PARAMETER
CYCLE    SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************
0 3        2.0758892E+02         1.0575000E+11  6.5250000E+02  1.6109484E+04
 NO REDUCTION IN SUM OF SQUARES. RESCALE PARAMETERS
 RESTRAINED CHANGE MECHANISM SETAT ( 0.5000E-01+ 0.4000) TIMES THE VALUE OF THE ORIGINAL PARAMETER
CYCLE    SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************
0 3        2.0731441E+02         1.1332500E+11  7.1775000E+02  1.6107582E+04
 NO REDUCTION IN SUM OF SQUARES. RESCALE PARAMETERS
 RESTRAINED CHANGE MECHANISM SETAT ( 0.2500E-01+ 0.4000) TIMES THE VALUE OF THE ORIGINAL PARAMETER
CYCLE    SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************
0 3        2.0721779E+02         1.2161250E+11  7.5037500E+02  1.6108631E+04
 NO REDUCTION IN SUM OF SQUARES. RESCALE PARAMETERS
 RESTRAINED CHANGE MECHANISM SETAT ( 0.1250E-01+ 0.4000) TIMES THE VALUE OF THE ORIGINAL PARAMETER
CYCLE    SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************
0 3        2.0717542E+02         1.2425625E+11  7.6668750E+02  1.6108155E+04
 PARTITION LESS THAN MESH LIMIT - - -                          RECYCLE RESTRAINT MECHANISM
CYCLE    SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************
0 4        2.1380205E+02        -1.2890001E+11 -7.8300000E+02  1.6120897E+04
 NO REDUCTION IN SUM OF SQUARES. RESCALE PARAMETERS
 RESTRAINED CHANGE MECHANISM SETAT ( 0.4000E+00+ 0.4000) TIMES THE VALUE OF THE ORIGINAL PARAMETER
CYCLE    SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************
0 4        2.5721825E+02        -4.2300015E+10 -2.6100000E+02  1.6113288E+04
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 NO REDUCTION IN SUM OF SQUARES. RESCALE PARAMETERS
 RESTRAINED CHANGE MECHANISM SETAT ( 0.2000E+00+ 0.8000) TIMES THE VALUE OF THE ORICINAL PARAMETER
CYCLE     SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************
0 4         1.0302211E+03         0.0000000E+00  0.0000000E+00  1.8109484E+04
 NO REDUCTION IN SUM OF SQUARES. RESCALE PARAMETERS
 RESTRAINED CHANGE MECHANISM SETAT ( 0.1000E+00+ 0.8000) TIMES THE VALUE OF THE ORIGINAL PARAMETER
CYCLE     SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************
0 4         2.4509721E+02         2.1149991E+10  1.3050000E+02  1.8107582E+04
 NO REDUCTION IN SUM OF SQUARES. RESCALE PARAMETERS
 RESTRAINED CHANGE MECHANISM SETAT ( 0.5000E-01+ 0.8000) TIMES THE VALUE OF THE ORIGINAL PARAMETER
CYCLE     SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************
0 4         2.2527654E+02         3.1724995E+10  1.9575000E+02  1.8106831E+04
 NO REDUCTION IN SUM OF SQUARES. RESCALE PARAMETERS
 RESTRAINED CHANGE MECHANISM SETAT ( 0.2500E-01+ 0.8000) TIMES THE VALUE OF THE ORIGINAL PARAMETER
CYCLE     SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************
0 4         2.2040263E+02         3.7012505E+10  2.2837500E+02  1.8106155E+04
 NO REDUCTION IN SUM OF SQUARES. RESCALE PARAMETERS
 RESTRAINED CHANGE MECHANISM SETAT ( 0.1250E-01+ 0.8000) TIMES THE VALUE OF THE ORIGINAL PARAMETER
CYCLE     SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************
0 4         2.1859171E+02         3.9856243E+10  2.4688750E+02  1.8105917E+04
 PARTITION LESS THAN MESH LIMIT - - -                          RECYCLE RESTRAINT MECHANISM
CYCLE     SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************
0 5         2.0848576E+02        -2.2726895E+11 -1.4986198E+03  1.8120897E+04
 NO REDUCTION IN SUM OF SQUARES. RESCALE PARAMETERS
 RESTRAINED CHANGE MECHANISM SETAT ( 0.1200E+01+ 1.8000) TIMES THE VALUE OF THE ORIGINAL PARAMETER
CYCLE     SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************
0 5         4.7882354E+02        -7.8834729E+09 -8.6809814E+01  1.8113288E+04
 NO REDUCTION IN SUM OF SQUARES. RESCALE PARAMETERS
 RESTRAINED CHANGE MECHANISM SETAT ( 0.6000E+00+ 1.8000) TIMES THE VALUE OF THE ORIGINAL PARAMETER
CYCLE     SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************
0 5         2.0824091E+02         1.0180827E+11  8.0409509E+02  1.8109484E+04
 NEW SQMIN=    2.082409E+02
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     I    B(I,3)          A(I,1)     A(I,2)     .....
0    1   5.124E-11       7.849E-20 -1.244E-11  5.951E-13
0    2  -8.402E-03      -1.244E-11  1.974E-03 -9.483E-05
0    3   5.035E-04       5.951E-13 -9.483E-05  5.984E-06

CYCLE     SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************

0 2          2.0624091E+02          1.0180827E+11  8.0409509E+02  1.61094L4E+04


     I    B(I,3)          A(I,1)     A(I,2)     .....
0    1  -3.402E+10       2.221E+22  1.421E+14  4.317E+13
0    2  -2.185E+02       1.421E+14  9.112E+05  3.103E+05
0    3   4.741E+00       4.317E+13  3.103E+05  7.939E+05

 S PARAMETERS

   1.0181E+11 -4.0723E+10 -3.4021E+10 -1.0000E+00
   8.0410E+02 -2.4164E+02 -2.1849E+02 -1.0000E+00
   1.6109E+04  6.4438E+03  4.7406E+00  1.0000E+00

CYCLE     SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************

0 3          2.0620749E+02          6.7787812E+10  3.8580095E+02  1.6114225E+04
 NEW SQMIN=    2.062075E+02


     I    B(I,3)          A(I,1)     A(I,2)     .....
0    1  -4.098E-11       1.805E-19 -2.893E-11  9.185E-13
0    2   7.145E-03      -2.893E-11  4.641E-03 -1.480E-04
0    3  -3.134E-04       9.185E-13 -1.480E-04  6.124E-06

CYCLE     SUM OF SQUARES        ********************************* B(J) PARAMETERS  ***************************** ***

0 3          2.0620749E+02          6.7787812E+10  3.8580095E+02  1.6114225E+04


     I    B(I,3)          A(I,1)     A(I,2)     .....
0    1   1.355E+10       4.249E+21  2.705E+13  1.803E+13
0    2   8.587E+01       2.705E+13  1.732E+05  1.375E+05
0    3  -3.422E+00       1.803E+13  1.375E+05  7.888E+05

 S PARAMETERS

   6.7788E+10  2.7115E+10  1.3549E+10  1.0000E+00
   3.8580E+02  1.5424E+02  8.5872E+01  1.0000E+00
   1.6114E+04 -6.4457E+03 -3.4224E+00 -1.0000E+00

CYCLE     SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************

0 4          2.0615884E+02          6.1336738E+10  4.7147275E+02  1.6110802E+04
 NEW SQMIN=    2.061588E+02


     I    B(I,3)          A(I,1)     A(I,2)     .....
0    1  -5.702E-12       1.247E-19 -1.992E-11  7.574E-13
0    2   8.928E-04      -1.992E-11  3.184E-03 -1.218E-04
0    3  -2.833E-05       7.574E-13 -1.218E-04  6.089E-06

CYCLE     SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************
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0 4          2.0815884E+02          8.1336738E+10  4.7147275E+02  1.8110802E+04

     I    B(I,3)          A(I,1)      A(I,2)     .....
0    1  -8.870E+08       8.838E+21  5.630E+13  2.854E+13
0    2  -5.212E+00       5.630E+13  3.599E+05  1.961E+05
0    3   1.456E+00       2.854E+13  1.961E+05  7.878E+05

 S PARAMETERS

  8.1337E+10 -3.2535E+10 -8.8695E+08 -1.0000E+00
  4.7147E+02 -1.8859E+02 -5.2117E+00 -1.0000E+00
  1.8111E+04  8.4443E+03  1.4581E+00  1.0000E+00

CYCLE     SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************

0 5          2.0815862E+02          8.0449782E+10  4.6626105E+02  1.8112258E+04
 NEW SQMIN=    2.081588E+02


     I    B(I,3)          A(I,1)      A(I,2)     .....
0    1   8.630E-14       1.273E-19 -2.032E-11  7.651E-13
0    2  -5.760E-08      -2.032E-11  3.247E-03 -1.229E-04
0    3  -1.292E-08       7.651E-13 -1.229E-04  8.084E-06

CYCLE     SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************

0 5          2.0815862E+02          8.0449782E+10  4.6626105E+02  1.8112258E+04


     I    B(I,3)          A(I,1)      A(I,2)     .....
0    1   2.173E+08       8.481E+21  5.406E+13  2.598E+13
0    2   1.343E+00       5.406E+13  3.460E+05  1.925E+05
0    3  -4.054E-01       2.598E+13  1.925E+05  7.890E+05

 S PARAMETERS

  8.0450E+10  3.2180E+10  2.1732E+08  1.0000E+00
  4.6626E+02  1.8650E+02  1.3430E+00  1.0000E+00
  1.8112E+04 -8.4449E+03 -4.0542E-01 -1.0000E+00

CYCLE     SUM OF SQUARES        ********************************* B(J) PARAMETERS  *********************************

0 6          2.0815857E+02          8.0687099E+10  4.6760410E+02  1.8111853E+04

C. Termination Code

 NEGLIGIBLE CHANGE IN SUM OF SQUARES

C. Document number of iterations and fit

     AFTER    6 ITERATIONS
        THE MINIMIZING VALUES OF THE PARAMETERS ARE:
  8.0687099E+10  4.6760410E+02  1.8111853E+04

     WITH THE FOLLOWING STD. DEVIATIONS:
  9.8831018E+10  8.3123511E+02  9.5323285E+02


  THE SUM OF SQUARES,VARIANCE AND SAMPLE STD. DEVIATION FOR THIS FIT ARE      2.08159E+02      1.15172E+00      1.07318E+00
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C. Pointwise Comparisons

NUMBER	LABEL		Y OBSERVED	Y CALCULATED	OBS-CALC	(OBS-CALC)/OBS
1	AGC	P530	2.06200E+01	1.84909E+02	-1.64289E+02	-7.96746E+00
2	AGC	P531	1.11100E+01	1.68320E+02	-1.57210E+02	-1.41503E+01
3	AGC	P532	1.26500E+01	1.68320E+02	-1.55670E+02	-1.23059E+01
4	AGC	P533	1.03600E+01	1.68320E+02	-1.57960E+02	-1.52471E+01
5	AGC	P534	1.21500E+01	1.68320E+02	-1.56170E+02	-1.28535E+01
6	AGC	P535	1.33200E+01	1.68320E+02	-1.55000E+02	-1.16367E+01
7	AGC	P536	1.52500E+01	1.75178E+02	-1.59928E+02	-1.04870E+01
8	AGC	P537	1.69100E+01	1.68981E+02	-1.52171E+02	-9.05240E+00
9	AGC	P538	1.62300E+01	1.68981E+02	-1.52751E+02	-9.41163E+00
10	AGC	P539	1.67100E+01	1.68981E+02	-1.52271E+02	-9.11255E+00
11	AGC	P540	1.89400E+01	1.84909E+02	-1.65969E+02	-8.76288E+00
12	AGC	P541	1.84500E+01	1.68981E+02	-1.50531E+02	-8.15885E+00
13	AGC	P542	1.30900E+01	1.68981E+02	-1.55891E+02	-1.19092E+01
14	AGC	P543	1.30200E+01	1.75178E+02	-1.62158E+02	-1.24545E+01
15	AGC	P544	1.88200E+01	1.68981E+02	-1.50101E+02	-7.95025E+00
16	OGC	P545	2.85300E+01	1.68846E+02	-1.42316E+02	-5.36436E+00
17	OGC	P546	2.17400E+01	1.68846E+02	-1.47106E+02	-6.76862E+00
18	OGC	P547	2.76000E+01	1.75143E+02	-1.47543E+02	-5.34577E+00
19	OGC	P548	2.81800E+01	1.84630E+02	-1.56450E+02	-5.55180E+00
20	OGC	P549	2.65500E+01	1.68846E+02	-1.42298E+02	-5.35956E+00
21	OGC	P550	2.03400E+01	1.68846E+02	-1.38506E+02	-4.56514E+00
22	OGC	P551	2.41100E+01	1.68846E+02	-1.44738E+02	-6.00317E+00
23	OGC	P552	1.49400E+01	1.75143E+02	-1.60203E+02	-1.07231E+01
24	OGC	P553	2.12900E+01	1.68846E+02	-1.47556E+02	-6.93079E+00
25	OGC	P554	2.63100E+01	1.84630E+02	-1.58320E+02	-6.01748E+00
26	OGC	P555	2.34300E+01	1.68846E+02	-1.45416E+02	-6.20642E+00
27	OGC	P556	2.17900E+01	1.68846E+02	-1.47056E+02	-6.74880E+00
28	OGC	P557	2.88900E+01	1.68846E+02	-1.40156E+02	-4.85520E+00
29	IC1	P515	2.94100E+01	1.84412E+02	-1.55002E+02	-5.27039E+00
30	IC1	P516	1.63100E+01	1.77607E+02	-1.61297E+02	-9.88947E+00
31	IC1	P517	1.43600E+01	1.72135E+02	-1.57775E+02	-1.09871E+01
32	IC1	P519	1.54400E+01	1.69463E+02	-1.54023E+02	-9.97558E+00
33	IC1	P520	1.16000E+01	1.72135E+02	-1.60535E+02	-1.38392E+01
34	IC1	P521	1.25300E+01	1.69463E+02	-1.56933E+02	-1.25246E+01
35	IC1	P522	1.02300E+01	1.72135E+02	-1.61905E+02	-1.58285E+01
36	IC1	P523	1.26600E+01	1.69463E+02	-1.56803E+02	-1.23857E+01
37	IC1	P529	1.36700E+01	1.84412E+02	-1.70742E+02	-1.24903E+01
38	XS2A	P850	4.83700E+02	2.07635E+02	2.76065E+02	5.70735E-01
39	XS2A	P852	4.29300E+02	2.07635E+02	2.21665E+02	5.16340E-01
40	XS2A	P853	4.88100E+02	2.07635E+02	2.80465E+02	5.74605E-01
41	XS2A	P865	4.99000E+02	2.07635E+02	2.91365E+02	5.83897E-01
42	XS2A	P870	4.89600E+02	2.07635E+02	2.81965E+02	5.57848E-01
43	XS2A	P874	4.42200E+02	2.07635E+02	2.34565E+02	5.30449E-01
44	XS2B	P839	4.96900E+02	2.40888E+02	2.56012E+02	5.15219E-01
45	XS2B	P848	5.65800E+02	2.40888E+02	3.24712E+02	5.74102E-01
46	XS2B	P858	5.37700E+02	2.40888E+02	2.96812E+02	5.52003E-01
47	XS2B	P880	5.89200E+02	2.40888E+02	3.48312E+02	5.91161E-01
48	XS2B	P873	4.82800E+02	2.40888E+02	2.41912E+02	5.01081E-01
49	XS2B	P887	5.34000E+02	2.40888E+02	2.93112E+02	5.48899E-01
50	XS2C	P835	6.87300E+02	3.38095E+02	3.49205E+02	5.08082E-01
51	XS2C	P844	6.46300E+02	3.38095E+02	3.08205E+02	4.76876E-01
52	XS2C	P862	6.56300E+02	3.38095E+02	3.18205E+02	4.84847E-01
53	XS2C	P866	6.69400E+02	3.38095E+02	3.31305E+02	4.94928E-01
54	XS2C	P867	6.60500E+02	3.38095E+02	3.22405E+02	4.88122E-01

55	XS2C	P872	6.91200E+02	3.38095E+02	3.53205E+02	5.10929E-01
56	XS2D	P842	6.64800E+02	4.09025E+02	2.55575E+02	3.84555E-01
57	XS2D	P845	7.39200E+02	4.09025E+02	3.30175E+02	4.46865E-01
58	XS2D	P851	6.15100E+02	4.09025E+02	2.06075E+02	3.35027E-01
59	XS2D	P859	5.19500E+02	4.09025E+02	1.10475E+02	2.12657E-01
60	XS2D	P869	6.26700E+02	4.09025E+02	2.17675E+02	3.47335E-01
61	XS2D	P888	6.22200E+02	4.09025E+02	2.13175E+02	3.42815E-01
62	XS2E	P843	6.21400E+02	4.94834E+02	1.26566E+02	2.03878E-01
63	XS2E	P858	7.47400E+02	4.94834E+02	2.52566E+02	3.37926E-01
64	XS2E	P881	5.96300E+02	4.94834E+02	1.01466E+02	1.70159E-01
65	XS2E	P888	5.88900E+02	4.94834E+02	9.40658E+01	1.59731E-01
66	XS2E	P879	6.15800E+02	4.94834E+02	1.20966E+02	1.96437E-01
67	XS2E	P885	8.06500E+02	4.94834E+02	3.11866E+02	3.86442E-01
68	XS3EE	P837	4.15900E+02	3.15299E+02	1.00601E+02	2.41888E-01
69	XS3EE	P841	4.07900E+02	3.15299E+02	9.26010E+01	2.27019E-01
70	XS3EE	P854	4.20800E+02	3.15299E+02	1.05501E+02	2.50715E-01
71	XS3EE	P855	4.63700E+02	3.15299E+02	1.48401E+02	3.20037E-01
72	XS3EE	P871	4.05200E+02	3.15299E+02	8.99011E+01	2.21868E-01
73	XS3EE	P878	4.26300E+02	3.15299E+02	1.11001E+02	2.60382E-01
74	XS3F	P838	7.77000E+02	5.00815E+02	2.76385E+02	3.55708E-01
75	XS3F	P847	7.93300E+02	5.00815E+02	2.92685E+02	3.68946E-01
76	XS3F	P848	6.99800E+02	5.00815E+02	1.98985E+02	2.84427E-01
77	XS3F	P876	6.25800E+02	5.00815E+02	1.24985E+02	1.99785E-01
78	XS3F	P888	5.58000E+02	5.00815E+02	5.53853E+01	9.98138E-02
79	XS3F	P890	6.92200E+02	5.00815E+02	1.91585E+02	2.76777E-01
80	XS3G	P836	5.41600E+02	3.51047E+02	1.90553E+02	3.51833E-01
81	XS3G	P840	6.68300E+02	3.51047E+02	3.17253E+02	4.74718E-01
82	XS3G	P863	5.68200E+02	3.51047E+02	2.17153E+02	3.82177E-01
83	XS3G	P864	7.21600E+02	3.51047E+02	3.70553E+02	5.13518E-01
84	XS3G	P880	6.54000E+02	3.51047E+02	3.02953E+02	4.63231E-01
85	XS3G	P882	5.37800E+02	3.51047E+02	1.86753E+02	3.47253E-01
86	XS3H	P849	8.21200E+02	5.13791E+02	3.07409E+02	3.74342E-01
87	XS3H	P875	6.53600E+02	5.13791E+02	1.39809E+02	2.13906E-01
88	XS3H	P877	5.28200E+02	5.13791E+02	1.44093E+01	2.72800E-02
89	XS3H	P883	8.07900E+02	5.13791E+02	2.94109E+02	3.64042E-01
90	XS3H	P884	5.94200E+02	5.13791E+02	8.04093E+01	1.35324E-01
91	XS3H	P889	5.88100E+02	5.13791E+02	7.43093E+01	1.26355E-01
92	XS4E	Q433	1.20700E+01	1.86593E+02	-1.74523E+02	-1.44592E+01
93	XS4E	Q489	1.25600E+01	1.86593E+02	-1.74033E+02	-1.38561E+01
94	XS4E	Q493	1.08000E+01	1.83593E+02	-1.75793E+02	-1.62771E+01
95	XS4E	Q505	6.35500E+00	1.86593E+02	-1.78236E+02	-2.13331E+01
96	XS4H	Q369	7.27600E+02	3.51137E+02	3.78463E+02	5.17404E-01
97	XS4H	Q525	5.53800E+02	3.51137E+02	2.02663E+02	3.65950E-01
98	XS4H	Q598	4.91100E+02	3.51137E+02	1.39963E+02	2.84999E-01
99	XS4H	Q609	5.36300E+02	3.51137E+02	1.85163E+02	3.45260E-01
100	GC1	Q387	8.11600E+02	1.09244E+03	-2.80841E+02	-3.46034E-01
101	GC1	Q389	8.46000E+02	1.09244E+03	-2.48441E+02	-2.91301E-01
102	GC1	Q390	7.97800E+02	1.05188E+03	-2.54077E+02	-3.18472E-01
103	GC1	Q391	7.57800E+02	1.05188E+03	-2.94077E+02	-3.88067E-01
104	GC2	Q383	1.15700E+03	1.09820E+03	5.88019E+01	5.08227E-02
105	GC2	Q384	1.13300E+03	1.09820E+03	3.48019E+01	3.07166E-02
106	GC2	Q385	1.04800E+03	1.04838E+03	-3.58079E-01	-3.39770E-04
107	GC2	Q388	1.04200E+03	1.04838E+03	-8.35808E+00	-8.09885E-03
108	GC2	Q370	9.37300E+02	1.01860E+03	-8.13040E+01	-8.67427E-02
109	GC2	Q371	9.47900E+02	1.01860E+03	-7.07039E+01	-7.45901E-02
110	GC3	Q398	4.52500E+01	1.50578E+02	-1.05328E+02	-2.32769E+00
111	GC3	Q399	6.82400E+01	1.50578E+02	-8.23379E+01	-1.20659E+00
112	GC3	Q396	5.72900E+01	1.44950E+02	-8.76605E+01	-1.53012E+00
113	GC3	Q397	3.90800E+01	1.44950E+02	-1.05890E+02	-2.71097E+00
114	GC3	Q394	5.62600E+01	1.39521E+02	-8.32814E+01	-1.47994E+00
115	GC3	Q395	5.63900E+01	1.39521E+02	-8.31314E+01	-1.47422E+00
116	GC4	Q405	8.79700E+02	7.08080E+02	-2.63804E+01	-3.87824E-02

117	GC4	Q406	8.95500E+02	7.06060E+02	-1.05804E+01	-1.51839E-02
118	GC4	Q403	9.42100E+02	8.79598E+02	2.62504E+02	2.78637E-01
119	GC4	Q404	9.16500E+02	8.79598E+02	2.38904E+02	2.58488E-01
120	GC5	Q497	2.80200E+01	8.18378E+01	-5.38178E+01	-1.92069E+00
121	GC5	Q499	3.37300E+01	8.18378E+01	-4.81078E+01	-1.42626E+00
122	GC5	Q495	2.95500E+01	7.88338E+01	-4.90838E+01	-1.66104E+00
123	GC5	Q498	2.80200E+01	7.88338E+01	-5.25538E+01	-2.01510E+00
124	GC6	Q517	1.84800E+02	1.90770E+02	-2.59700E+01	-1.57585E-01
125	GC6	Q519	1.52100E+02	1.90770E+02	-3.86700E+01	-2.54241E-01
126	GC7	Q513	4.21200E+02	2.70885E+02	1.50315E+02	3.56874E-01
127	GC7	Q514	4.14500E+02	2.70885E+02	1.43815E+02	3.48478E-01
128	GC8	Q512	7.93300E+02	1.12798E+03	-3.34685E+02	-4.21889E-01
129	GC8	Q490	5.88000E+02	1.11387E+03	-5.25667E+02	-8.93591E-01
130	GC9	Q520	2.24400E+02	2.21545E+02	2.85303E+00	1.27229E-02
131	GC9	Q522	2.45900E+02	2.21545E+02	2.43550E+01	9.90444E-02
132	GC10	Q509	5.64900E+02	1.11335E+03	-5.48453E+02	-9.70885E-01
133	GC12	Q503	1.45700E+03	1.11335E+03	3.43647E+02	2.35859E-01
134	GC13X	Q533	5.40900E+02	1.11323E+03	-5.72328E+02	-1.05810E+00
135		Q539	1.92600E+03	1.11323E+03	8.12710E+02	4.21968E-01
136		Q535	1.30000E+01	1.87973E+02	-1.74973E+02	-1.34594E+01
137		T502	5.97900E+01	1.87973E+02	-1.28183E+02	-2.14388E+00
138		Q536	1.11700E+01	1.87973E+02	-1.76803E+02	-1.58284E+01
139		T515	5.69400E+01	1.87973E+02	-1.31033E+02	-2.30124E+00
140		Q537	2.87800E+01	1.87973E+02	-1.59193E+02	-5.53137E+00
141		T517	6.14000E+01	1.87973E+02	-1.26573E+02	-2.06145E+00
142	ES1	Q384	7.32000E+00	1.77541E+02	-1.70221E+02	-2.32542E+01
143	ES1	Q385	1.01600E+01	1.77541E+02	-1.67381E+02	-1.64745E+01
144	ES1	Q386	1.03100E+01	1.77541E+02	-1.67231E+02	-1.62203E+01
145	ES2	Q410	5.35000E+01	3.33284E+01	-2.01716E+01	3.77040E-01
146	ES2	Q411	5.54600E+01	3.33284E+01	2.21316E+01	3.99058E-01
147	ES2	Q426	6.76800E+01	3.33284E+01	3.43517E+01	5.07580E-01
148	ES2	R967	4.34400E+01	3.33284E+01	1.01116E+01	2.32773E-01
149	ES2	R972	4.54600E+01	3.33284E+01	1.21316E+01	2.66884E-01
150	ES2	R979	2.88200E+01	3.33284E+01	-4.50835E+00	-1.56431E-01
151	ES8	Q414	4.89100E+02	2.94767E+02	1.94333E+02	3.97328E-01
152	ES8	Q416	5.59600E+02	2.94767E+02	2.64833E+02	4.73254E-01
153	ES8	Q422	3.88300E+02	2.94767E+02	9.35330E+01	2.40878E-01
154	ES8	Q431	2.47500E+01	1.77611E+02	-1.52861E+02	-6.17820E+00
155	ES8	Q432	2.07800E+01	1.77611E+02	-1.56851E+02	-7.55544E+00
156	ES8	Q436	4.43000E+00	1.77611E+02	-1.73181E+02	-3.90928E+01
157	ES8A	Q452	1.76900E+01	1.77700E+02	-1.60010E+02	-9.04522E+00
158	ES8A	Q481	2.51800E+01	1.77700E+02	-1.52540E+02	-6.06280E+00
159	ES8A	Q469	1.88800E+01	1.77700E+02	-1.58840E+02	-8.42206E+00
160	ES10	Q434	7.83000E+00	1.84873E+01	-1.06573E+01	-1.36108E+00
161	ES10	Q435	8.78000E+00	1.84873E+01	-9.70730E+00	-1.10581E+00
162	ES10	Q438	8.37000E+00	1.84873E+01	-1.01173E+01	-1.20876E+00
163	ES14	Q455	6.33000E+00	1.77700E+02	-1.71370E+02	-2.70727E+01
164	ES14	Q460	6.67000E+00	1.77700E+02	-1.71030E+02	-2.56417E+01
165	ES14	Q467	8.15000E+00	1.77700E+02	-1.69550E+02	-2.08037E+01
166	ES16	Q444	3.09000E+00	1.84873E+01	-1.53973E+01	-4.98294E+00
167	ES16	Q456	3.08000E+00	1.84873E+01	-1.54073E+01	-5.00237E+00
168	ES16	Q483	2.90000E+00	1.84873E+01	-1.55873E+01	-5.37490E+00
169	ES18	Q450	1.07800E+02	7.55494E+02	-6.47894E+02	-6.00829E+00
170	ES18	Q451	8.94300E+01	7.55494E+02	-6.66064E+02	-7.44788E+00
171	ES18	Q453	8.08300E+01	7.55494E+02	-6.74864E+02	-8.34670E+00
172	ES20	Q472	4.22000E+02	2.01500E+02	2.20500E+02	5.22511E-01
173	ES20	Q473	3.35000E+02	2.01500E+02	1.33500E+02	3.98507E-01
174	ES20	Q476	3.20300E+02	2.01500E+02	1.18800E+02	3.70901E-01
175	ES22	Q481	1.18300E+01	2.14035E+01	-9.57351E+00	-8.09257E-01
176	ES22	Q484	1.65100E+01	2.14035E+01	-4.89351E+00	-2.96397E-01
177	ES22	Q485	1.09000E+01	2.14035E+01	-1.05035E+01	-9.63625E-01
178	ES24	Q483	8.81700E+02	8.45374E+02	3.63257E+01	4.11996E-02

179	ES24	Q486	8.83200E+02	8.45374E+02	3.78257E+01	4.28280E-02
180	ES24	Q4..	9.50000E+02	8.45374E+02	1.04626E+02	1.10132E-01
181	ES24	Q690	6.25000E+02	8.45374E+02	-2.19474E+02	-3.50854E-01
182	ES24	T 53	6.68600E+02	8.45374E+02	-1.76774E+02	-2.64395E-01

AVERAGE DEVIATION	2.09539E+00	
AVERAGE REL DEV	-3.82953E+00	
AVE ABS REL DEV	4.13689E+00	
MAXIMUM DEVIATION	8.12710E+02	AT POINT 135
MAXIMUM REL DEV	3.90928E+01	AT POINT 158
ROOT MEAN SQUARE DEVIATION	1.07318E+00	

CAUCHY CONVERGENCE OF SUM OF SQUARES. FRACTIONAL REDUCTION IN MINIMUM SUMSQ IS LESS THAN 5.000E-07

C. Output from the uncertainty propagation routine ERPROP
C. Zero in fourth column indicates benchmark (MBD only) fit.

TIME YRS	DEPTH MICRONS	UNCERTAINTY MICRONS	
1.000E+00	7.332791E+02	7.393943E+01	0.000000E+00
2.000E+00	1.411601E+03	2.010527E+02	0.000000E+00
5.000E+00	3.227600E+03	7.234831E+02	0.000000E+00
1.000E+01	5.629428E+03	1.678392E+03	0.000000E+00
2.000E+01	9.084351E+03	3.438128E+03	0.000000E+00
5.000E+01	1.376238E+04	6.495685E+03	0.000000E+00
1.000E+02	1.709013E+04	9.091291E+03	0.000000E+00
2.000E+02	2.010962E+04	1.178257E+04	0.000000E+00
3.000E+02	2.229156E+04	1.383987E+04	0.000000E+00
5.000E+02	2.511629E+04	1.668513E+04	0.000000E+00
1.000E+03	2.928119E+04	2.111937E+04	0.000000E+00

C. Begin Sequential Evaluations, proceed in originally-generated order through the ESS, 1-32

PHASE 2 ** EVALUATING EXPERIMENT NUMBER: 1

ADDED VIRTUAL DATA POINT: [V 1- 11111]
Y,E= 4.783800 81.92543
C.
C. The iterations and pointwise comparisons appear here
C.

AVERAGE DEVIATION	2.09987E+00	
AVERAGE REL DEV	-3.80864E+00	
AVE ABS REL DEV	4.11435E+00	
MAXIMUM DEVIATION	8.12831E+02	AT POINT 135
MAXIMUM REL DEV	3.90935E+01	AT POINT 158
ROOT MEAN SQUARE DEVIATION	1.07020E+00	

CAUCHY CONVERGENCE OF SUM OF SQUARES. FRACTIONAL REDUCTION IN MINIMUM SUMSQ IS LESS THAN 5.000E-07

TIME YRS	DEPTH MICRONS	UNCERTAINTY MICRONS	
1.000E+00	7.331759E+02	7.391483E+01	2.458717E-02
2.000E+00	1.411393E+03	2.012343E+02	-1.815948E-01
5.000E+00	3.227085E+03	7.247404E+02	-1.257263E+00
1.000E+01	5.628467E+03	1.681752E+03	-3.359819E+00
2.000E+01	9.082682E+03	3.445465E+03	-7.337158E+00
5.000E+01	1.375963E+04	6.509926E+03	-1.428172E+01
1.000E+02	1.708657E+04	9.111388E+03	-2.009688E+01
2.000E+02	2.010517E+04	1.178860E+04	-2.603418E+01

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   3.000E+02   2.228648E+04   1.387051E+04  -3.063985E+01
   5.000E+02   2.511036E+04   1.672204E+04  -3.690820E+01
   1.000E+03   2.925388E+04   2.118597E+04  -4.680742E+01

 PHASE 2 ** EVALUATING EXPERIMENT NUMBER:     2

 ADDED VIRTUAL DATA POINT:   [ V    2- 21111]
 Y,E=   1327.772       285.7686

C.
C.
C. This continues to virtual data point [V   32- 22222]
C.
C.

PHASE 2 ** EVALUATING EXPERIMENT NUMBER:    32

 ADDED VIRTUAL DATA POINT:   [ V   32- 22222]
 Y,E=   7420.588       278.1803

 NEGLIGIBLE CHANGE IN SUM OF SQUARES

     AFTER    1 ITERATIONS
        THE MINIMIZING VALUES OF THE PARAMETERS ARE:
  8.0608428E+10  4.6725801E+02  1.6112378E+04

     WITH THE FOLLOWING STD. DEVIATIONS:
  3.0414799E+10  1.8115343E+02  8.1524707E+02


  THE SUM OF SQUARES,VARIANCE AND SAMPLE STD. DEVIATION FOR THIS FIT ARE     2.08158E+02     1.14532E+00     1.07020E+00


   2.000E+00   1.411548E+03   4.715290E+01   1.538998E+02
   5.000E+00   3.227325E+03   1.211424E+02   6.023407E+02
   1.000E+01   5.628716E+03   2.908677E+02   1.387525E+03
   2.000E+01   9.082788E+03   6.447813E+02   2.793336E+03
   5.000E+01   1.375934E+04   1.305315E+03   5.190349E+03
   1.000E+02   1.708588E+04   1.886223E+03   7.205068E+03
   2.000E+02   2.010398E+04   2.495871E+03   9.266896E+03
   3.000E+02   2.228488E+04   2.976818E+03   1.086305E+04
   5.000E+02   2.510820E+04   3.640922E+03   1.304421E+04
   1.000E+03   2.925088E+04   4.884534E+03   1.843483E+04

C.
C. Now the ESS data is reordered by greatest-to-least uncertainty reduction
C.
      Point     Delta Uncert.  Delta Unc./BMark Unc.

   32- 22222   1.086305E+04   7.849100E-01
   24- 22212   1.079574E+04   7.800467E-01
   30- 21222   1.068224E+04   7.718457E-01
   22- 21212   1.061822E+04   7.670755E-01
   28- 22122   2.611241E+03   1.886753E-01
   20- 22112   2.462118E+03   1.779004E-01
   26- 21122   2.237070E+03   1.616396E-01
   18- 21112   2.114595E+03   1.527901E-01
   12- 22121   3.995605E+02   2.887026E-02
    4- 22111   3.806426E+02   2.750334E-02
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   10- 21121   3.248887E+02   2.347484E-02
    2- 21111   3.002852E+02   2.169711E-02
   31- 12222   2.953809E+02   2.134275E-02
   23- 12212   2.077959E+02   1.501430E-02
   29- 11222   1.266318E+02   9.149788E-03
   21- 11212   1.142002E+02   8.251539E-03
    8- 22211   3.544922E-01   2.561384E-05
   16- 22221  -4.687500E-01  -3.386955E-05
   14- 21221  -1.599609E+00  -1.155798E-04
    6- 21211  -1.644531E+00  -1.188257E-04
   15- 12221  -2.449023E+01  -1.769543E-03
   13- 11221  -2.829688E+01  -2.044592E-03
   27- 12122  -2.833887E+01  -2.047626E-03
   25- 11122  -2.861328E+01  -2.067454E-03
   19- 12112  -2.879492E+01  -2.080578E-03
    3- 12111  -2.978320E+01  -2.151986E-03
   17- 11112  -3.009277E+01  -2.174354E-03
   11- 12121  -3.048828E+01  -2.202932E-03
    9- 11121  -3.061719E+01  -2.212248E-03
    1- 11111  -3.063965E+01  -2.213869E-03
    7- 12211  -3.549219E+01  -2.564489E-03
    5- 11211  -3.737402E+01  -2.700481E-03

C.
C. In phase 3 the previously ordered ESS is accumulated hence "added" versus "evaluated"
C.

 PHASE 3 *** ADDING EXPERIMENT NUMBER:     1

 ADDED VIRTUAL DATA POINT:    [ V   32- 22222]
 Y,E=   7420.582        278.1801


    1.000E+00   7.332707E+02   2.819351E+01   4.574592E+01
    2.000E+00   1.411548E+03   4.715280E+01   1.539001E+02
    5.000E+00   3.227324E+03   1.211432E+02   6.023399E+02
    1.000E+01   5.628714E+03   2.908690E+02   1.387523E+03
    2.000E+01   9.082793E+03   6.447934E+02   2.793334E+03
    5.000E+01   1.375933E+04   1.305322E+03   5.190342E+03
    1.000E+02   1.708584E+04   1.886228E+03   7.205083E+03
    2.000E+02   2.010386E+04   2.495881E+03   9.286887E+03
    3.000E+02   2.228486E+04   2.978828E+03   1.086304E+04
    5.000E+02   2.510817E+04   3.640937E+03   1.304420E+04
    1.000E+03   2.925084E+04   4.684550E+03   1.643481E+04


 PHASE 3 *** ADDING EXPERIMENT NUMBER:     2

 ADDED VIRTUAL DATA POINT:    [ V   24- 22212]
 Y,E=   7420.580        288.9709

87878787887
 CAUCHY CONVERGENCE OF SUM OF SQUARES.  FRACTIONAL REDUCTION IN MINIMUM SUMSQ IS LESS THAN  5.000E-07

 PHASE 3 *** ADDING EXPERIMENT NUMBER:    32

 ADDED VIRTUAL DATA POINT:    [ V    5- 11211]
 Y,E=   82.71988        117.0323

 NEGLIGIBLE CHANGE IN SUM OF SQUARES

     AFTER     1 ITERATIONS
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THE MINIMIZING VALUES OF THE PARAMETERS ARE:
8.0685887E+10 4.6758340E+02 1.6110374E+04

WITH THE FOLLOWING STD. DEVIATIONS:
1.0923618E+10 8.4830513E+01 4.3218503E+02

THE SUM OF SQUARES,VARIANCE AND SAMPLE STD. DEVIATION FOR THIS FIT ARE 2.06158E+02 9.77054E-01 9.88460E-01

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AVERAGE DEVIATION	1.81560E+00		
AVERAGE REL DEV	-3.25693E+00		
AVE ABS REL DEV	3.51837E+00		
MAXIMUM DEVIATION	8.12882E+02	AT POINT	135
MAXIMUM REL DEV	3.90937E+01	AT POINT	156
ROOT MEAN SQUARE DEVIATION	9.88460E-01		

CAUCHY CONVERGENCE OF SUM OF SQUARES. FRACTIONAL REDUCTION IN MINIMUM SUMSQ IS LESS THAN 5.000E-07

TIME YRS	DEPTH MICROMS	UNCERTAINTY MICROMS	
1.000E+00	7.331629E+02	8.987084E+00	6.495237E+01
2.000E+00	1.411375E+03	1.884575E+01	1.824070E+02
5.000E+00	3.227074E+03	5.954789E+01	6.639354E+02
1.000E+01	5.628495E+03	1.396898E+02	1.538702E+03
2.000E+01	9.082806E+03	2.936950E+02	3.144433E+03
5.000E+01	1.375995E+04	5.695652E+02	5.926100E+03
1.000E+02	1.708707E+04	8.079352E+02	8.283355E+03
2.000E+02	2.010586E+04	1.055910E+03	1.070688E+04
3.000E+02	2.228732E+04	1.249983E+03	1.258988E+04
5.000E+02	2.511142E+04	1.516995E+03	1.516814E+04
1.000E+03	2.925538E+04	1.935039E+03	1.918433E+04
32- 22222	1.086304E+04	7.849092E-01	
24- 22212	1.131993E+04	8.179219E-01	
30- 21222	1.149219E+04	8.303883E-01	
22- 21212	1.158825E+04	8.373095E-01	
28- 22122	1.165575E+04	8.421863E-01	
20- 22112	1.170498E+04	8.457439E-01	
26- 21122	1.174144E+04	8.483779E-01	
18- 21112	1.177105E+04	8.505175E-01	
12- 22121	1.178242E+04	8.513389E-01	
4- 22111	1.178848E+04	8.517753E-01	
10- 21121	1.179595E+04	8.523167E-01	
2- 21111	1.180579E+04	8.530277E-01	
31- 12222	1.180631E+04	8.532102E-01	
23- 12212	1.181358E+04	8.535908E-01	
29- 11222	1.181883E+04	8.539899E-01	
21- 11212	1.182405E+04	8.543470E-01	
8- 22211	1.235241E+04	8.925236E-01	
16- 22221	1.247579E+04	9.014388E-01	
14- 21221	1.252427E+04	9.049416E-01	
6- 21211	1.255232E+04	9.069685E-01	
15- 12221	1.255557E+04	9.072028E-01	
13- 11221	1.255877E+04	9.074342E-01	
27- 12122	1.258194E+04	9.078836E-01	
25- 11122	1.258510E+04	9.078917E-01	
19- 12112	1.258822E+04	9.081172E-01	
3- 12111	1.257132E+04	9.083412E-01	
17- 11112	1.257440E+04	9.085639E-01	

11- 12121	1.257747E+04	9.087858E-01
9- 11121	1.258051E+04	9.090051E-01
1- 11111	1.258390E+04	9.092500E-01
7- 12211	1.258690E+04	9.094667E-01
5- 11211	1.258988E+04	9.096824E-01

JADD = 1

TIME YRS	DEPTH MICROMS	UNCERTAINTY MICROMS	
1.000E+00	7.332664E+02	8.987194E+00	1.920632E+01
2.000E+00	1.411543E+03	1.864380E+01	2.850879E+01
5.000E+00	3.227324E+03	5.953369E+01	6.160953E+01
1.000E+01	5.628732E+03	1.396465E+02	1.512225E+02
2.000E+01	9.082851E+03	2.935822E+02	3.512112E+02
5.000E+01	1.375947E+04	5.692982E+02	7.360242E+02
1.000E+02	1.708604E+04	8.075104E+02	1.078718E+03
2.000E+02	2.010423E+04	1.055301E+03	1.440579E+03
3.000E+02	2.228518E+04	1.249218E+03	1.727810E+03
5.000E+02	2.510858E+04	1.516004E+03	2.124933E+03
1.000E+03	2.925135E+04	1.933871E+03	2.750879E+03
17- 22221	4.913547E+02	1.650598E-01	
16- 22211	5.716572E+02	1.920357E-01	
18- 21221	6.071611E+02	2.039824E-01	
1- 22212	1.207370E+03	4.055898E-01	
19- 21211	1.233710E+03	4.144377E-01	
2- 21222	1.485111E+03	4.988904E-01	
3- 21212	1.633325E+03	5.486798E-01	
4- 22122	1.639454E+03	5.507385E-01	
5- 22112	1.644854E+03	5.525523E-01	
6- 21122	1.649941E+03	5.542613E-01	
7- 21112	1.654835E+03	5.558383E-01	
20- 12221	1.658087E+03	5.569978E-01	
30- 12211	1.661498E+03	5.581436E-01	
21- 11221	1.664898E+03	5.592852E-01	
31- 11211	1.668277E+03	5.604210E-01	
9- 22111	1.674405E+03	5.624797E-01	
8- 22121	1.680247E+03	5.644421E-01	
10- 21121	1.685242E+03	5.661200E-01	
11- 21111	1.689924E+03	5.676929E-01	
12- 12222	1.693365E+03	5.688455E-01	
13- 12212	1.696715E+03	5.699741E-01	
14- 11222	1.699995E+03	5.710759E-01	
15- 11212	1.703232E+03	5.721634E-01	
24- 12112	1.706352E+03	5.732115E-01	
29- 11111	1.709454E+03	5.742538E-01	
28- 11121	1.712535E+03	5.752884E-01	
25- 12111	1.715592E+03	5.763155E-01	
22- 12122	1.718628E+03	5.773352E-01	
27- 12121	1.721648E+03	5.783497E-01	
26- 11112	1.724634E+03	5.793528E-01	
23- 11122	1.727610E+03	5.803527E-01	

JADD = 1

TIME YRS	DEPTH MICROMS	UNCERTAINTY MICROMS	
1.000E+00	7.332664E+02	8.987758E+00	8.178672E+00
2.000E+00	1.411543E+03	1.864518E+01	1.810906E+01
5.000E+00	3.227324E+03	5.953479E+01	6.060882E+01
1.000E+01	5.628732E+03	1.396476E+02	1.422246E+02
2.000E+01	9.082853E+03	2.935813E+02	2.989183E+02

5.000E+01	1.375947E+04	5.692932E+02	5.704571E+02
1.000E+02	1.708605E+04	8.075034E+02	8.047351E+02
2.000E+02	2.010423E+04	1.055291E+03	1.047010E+03
3.000E+02	2.228518E+04	1.249207E+03	1.236267E+03
5.000E+02	2.510857E+04	1.515989E+03	1.498070E+03
1.000E+03	2.925136E+04	1.933651E+03	1.901919E+03
3- 22212	5.699739E+02	2.293220E-01	
5- 21222	7.998251E+02	3.217999E-01	
6- 21212	9.323374E+02	3.751146E-01	
1- 22211	1.057440E+03	4.254481E-01	
2- 21221	1.110567E+03	4.468230E-01	
4- 21211	1.141875E+03	4.594595E-01	
7- 22122	1.148088E+03	4.619184E-01	
8- 22112	1.153486E+03	4.640909E-01	
9- 21122	1.158595E+03	4.661465E-01	
10- 21112	1.163195E+03	4.679972E-01	
16- 22121	1.169762E+03	4.706396E-01	
15- 22111	1.175474E+03	4.729378E-01	
17- 21121	1.180622E+03	4.750090E-01	
18- 21111	1.185408E+03	4.769344E-01	
19- 12222	1.188941E+03	4.783558E-01	
20- 12212	1.192399E+03	4.797471E-01	
21- 11222	1.195699E+03	4.810750E-01	
22- 11212	1.199034E+03	4.824167E-01	
11- 12221	1.202345E+03	4.837489E-01	
13- 11221	1.205556E+03	4.850409E-01	
12- 12211	1.208730E+03	4.863180E-01	
14- 11211	1.211891E+03	4.875897E-01	
29- 11112	1.215016E+03	4.888487E-01	
23- 12112	1.218112E+03	4.900924E-01	
25- 11121	1.221198E+03	4.913340E-01	
24- 11111	1.224255E+03	4.925643E-01	
27- 12122	1.227291E+03	4.937855E-01	
30- 11122	1.230222E+03	4.949650E-01	
26- 12111	1.233298E+03	4.962016E-01	
28- 12121	1.236267E+03	4.973969E-01	

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JADD = 6

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TIME YRS	DEPTH MICRONS	UNCERTAINTY MICRONS	
1.000E+00	7.332864E+02	8.987758E+00	5.983934E-01
2.000E+00	1.411543E+03	1.884516E+01	1.229395E+00
5.000E+00	3.227324E+03	5.953479E+01	4.200443E+00
1.000E+01	5.628732E+03	1.396478E+02	1.025105E+01
2.000E+01	9.082853E+03	2.935813E+02	2.196753E+01
5.000E+01	1.375947E+04	5.692932E+02	4.283923E+01
1.000E+02	1.708605E+04	8.075034E+02	6.083636E+01
2.000E+02	2.010423E+04	1.055291E+03	7.958289E+01
3.000E+02	2.228518E+04	1.249207E+03	9.429236E+01
5.000E+02	2.510857E+04	1.515989E+03	1.145521E+02
1.000E+03	2.925136E+04	1.933651E+03	1.463193E+02
1- 22122	6.111450E+00	4.548905E-03	
2- 22112	1.151111E+01	8.568007E-03	
3- 21122	1.682024E+01	1.237086E-02	
4- 21112	2.121997E+01	1.579456E-02	
5- 22121	2.778760E+01	2.068301E-02	
6- 22111	3.349988E+01	2.493480E-02	
7- 21121	3.864783E+01	2.876655E-02	
8- 21111	4.343323E+01	3.232844E-02	
9- 12222	4.696819E+01	3.495811E-02	

10-	12212	5.042419E+01	3.753199E-02
11-	11222	5.372473E+01	3.998866E-02
12-	11212	5.705945E+01	4.247078E-02
19-	11121	6.028552E+01	4.487203E-02
23-	12111	6.347546E+01	4.724638E-02
24-	12121	6.666405E+01	4.961228E-02
22-	11122	6.979736E+01	5.195193E-02
20-	11111	7.292334E+01	5.427867E-02
17-	11112	7.603174E+01	5.659233E-02
13-	12221	7.912524E+01	5.889490E-02
18-	12112	8.225342E+01	6.122328E-02
15-	12211	8.529626E+01	6.348815E-02
16-	11211	8.823401E+01	6.567478E-02
14-	11221	9.132251E+01	6.797364E-02
21-	12122	9.429239E+01	7.018416E-02

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