Sandia National Laboratories
Albuquerque, New Mexico 87185

March 15, 1988

Dr. Daniel Galson
Operations Branch
Division of High-Level Waste Management
Office of Nuclear Materials Safety
and Safeguards
U.S. Nuclear Regulatory Commission
Mail Stop 4D16
Washington, DC 20555

Dear Dr. Galson:

Enclosed is the February 1988 monthly report for FIN A1165. If you have any questions or comments, please feel free to contact me at (FTS) 844-8368, E. J. Bonano at (FTS)844-5303, or P. A. Davis at (FTS)846-5421.

This monthly report is late because of time spent by Sandia staff and management preparing and giving presentations to NRC staff and management on March 15 and 16.

Sincerely,

Robert M. Cranwell

Robert M. Cranwell, Supervisor
Waste Management Systems
Division 6416

RMC:6416

Enclosure

Copy to:
Office of the Director, NMSS
Attn: Program Support
Robert Browning, Director
Division of High-Level Waste Management
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A1165
WM-11
NH14

PROGRAM:	Licensing-Methodology Assistance		FIN A1165 Task I
CONTRACTOR:	Sandia National Laboratories	BUDGET PERIOD:	10/87 - 9/88
NMSS PROGRAM MANAGER:	D. Galson	BUDGET AMOUNT:	$248K
CONTRACT PROGRAM MANAGER:	R. M. Cranwell	FTS PHONE:	844-8368
PRINCIPAL INVESTIGATORS:	E. J. Bonano P. A. Davis	FTS PHONE: FTS PHONE:	844-5303 846-5421

PROJECT OBJECTIVE

To assist in the overall development and integration of the licensing assessment methodology.

ACTIVITIES DURING FEBRUARY 1988

E. Bonano and K. Wahi participated in a workshop at NRC on February 24 on Waste Package performance assessment. The main topic of discussion was the CONVO computer code developed by NRC consultants to simulate processes needed to assess compliance with the Waste Package Lifetime criterion in 10CFR60. The presentations focused on the mechanistic aspect of modeling these processes rather than the inner workings of the code. The processes discussed include (1) heat released from the waste form, (2) container corrosion (both uniform and pitting corrosion), (3) spent fuel and glass waste-form leaching, and (4) radionuclide transport through the packing. Other topics discussed include processes that may be important but are not yet included in the code; external, discrete, and unanticipated events; repository-scale (EBS) source-term modeling; and modifications needed to render the code applicable to the Yucca Mountain Site. Certain unresolved issues such as ground-water flow in tuff and zircaloy cladding corrosion were also discussed.

Based on Sandia's participation we make the following observations. One of the most attractive features of the methodology is the modular structure of the code. The fact that a PC version of the code (CONVOPC) is available makes it more accessible and easy to use. However, a major drawback of the PC version is that many simplifications had to be made. Some of these have to do with the use of very restrictive statistical procedures; for example, pdf's for uncertain variables being limited to uniform distributions. Other simplifications are concerned with treatment of a single waste package and the use of a linear interpolation scheme in the thermal response surface model, which may or may not be adequate. There are generic problems with both the PC and mainframe versions of the code. Some of these are related to the fact that some potentially important

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processes have not been accounted for; e. g., stress corrosion cracking, radiolysis-enhanced corrosion, thermoelastic stresses and strains and associated failure modes, radionuclide decay and decay chains in the transport model, and convective and radiative heat transfer. In addition, some of the approaches that they have implemented in the code may be inadequate and cause problems. Some specific examples are: (1) limited number of terms representing thermal decay for the long-term prediction of thermal output; (2) in the interest of computational efficiency, the use of less accurate numerical algorithms and analytic solutions which may not represent physical reality adequately; (3) the inability to describe time-dependent waste-form dissolution precludes sensitivity analyses for a major component that DOE may rely on to show compliance; (4) assumption of constant and spatially homogeneous thermal properties may not be appropriate because typically the packing has a lower thermal conductivity than the host rock, and the conductivity of some rocks seems to be a strong function of temperature; (5) the apparent inability to assign possible correlations between input variables; and (6) the single-waste package restriction in the PC version precludes determination of sensitivity with respect to important design variables such as canister spacing. For the most part, the user's manual for CONVOPC is very well written, thus making it easy for a new user to execute the code. We have obtained a copy of the code and have successfully run it on a PC. A major problem with the user's manual is the complete lack of sample problems so that a potential user could verify that the code has been properly installed and executed.

Subtask 1.1

I. Interim report: compilation of parameters and components of an overall licensing assessment methodology and development of a tracking scheme.

Most of the activity in this subtask during the month of February was associated with the preparation of this report. The following individuals worked on it: E. Bonano, P. Davis, I. Hall, C. Harlan, D. Gallegos, L. Paul, K. Wahi, M. Goodrich, and R. Guzowski. Each of these individuals had responsibilities to write one or more sections of the report following the outline forwarded to the NMSS PM with the January monthly progress report. These sections are to be turned in by March 4 when the assembly of the report is scheduled to commence. Preliminary assessments indicate that by the end of February the report was about 70 % complete. One of the major components of this report is the development of a tracking scheme for the licensing assessment methodology. Attached to this monthly progress report is a draft of the section on the tracking scheme. Another attachment to this monthly report is a preliminary list of the parameters used in codes and models identified so far.

II. Critical parameters and components for licensing assessment

Although there has not been formal activity in this report, we feel that the work on the interim report just described is directly related to preparing this formal report.

Subtask 1.2

I. Compilation, comparison, and evaluation of computer codes for licensing assessment

Work in this report follows directly from that for the reports in Subtask 1.1. As a result, in the preparation of the interim report discussed above, we have begun to identify some of the existing codes. Attached to this progress report is a peliminary list of ground-water flow codes.

Subtask 1.3

I. Modeling efforts needed to support a HLW repository license application

There has been no formal activity in this report; however, it is believed that its preparation follows directly from that in Subtask 1.1.

II. Processes for which validated models will not exist at the time of a HLW repository license application.

No activity.

III. Recommended approaches for evaluating the application of HLW disposal system models

No activity.

IV. Review of the NRC's modeling strategey document for HLW performance assessment

No activity.

V. A technical basis for NRC review of HLW repository modeling programs

No activity.

Subtask 1.4

I. Performance assessment program reviews

See discussion above on Waste Package performance assessment.

Management Issues

In the response to the January monthly progress report the NMSS PM requested a justification for the expenditures in this task. We have examined all budget reports for FY88 and believe that, with the exception of approximately 1 man-month of effort charged to this program, the expenditures are legitimate. One man-month of staff time was charged by error and the correction should be reflected in the monthly report for March. This would amount to approximately $9-10K of charges. Below we summarize the activities under this task.

R. Cranwell attended two one-week meetings of PAAG in Paris, France.

E. Bonano attended the one-week PSAC meeting in Paris, France and spent 4 days working on the associated trip report.

R. Cranwell, E. Bonano, and P. Davis attended a two-day meeting at DOE/HQ on Performance Allocation and Issue Resolution Strategy. In addition to the meeting, time was also charged for travel and reading of necessary documents and reports in preparation for the meeting.

E. Bonano and K. Wahi attended a one-day workshop at NRC on Waste Package performance assessment. Time charges include one day of travel and another day for reading associated documents.

Between E. Bonano and P. Davis, approximately 3 days a month are spent in the preparation of the monthly progress reports.

Approximately 4 man-months of staff time were spent during January and February working in the preparation of the interim report on the components of the licensing assessment methodology.

Total justified staff-time charges are approximately $52-53K.

Travel charges covering the travel in the aforementioned trips have amounted to approximately $3K.

Direct support charges for work done by Sandia's information services on the scenario selection and screening report are approximately $2K.

Contractor charges against this task are $7K covering time spent by staff of GRAM, Inc. (K. Wahi) and Remote Sensing (R. Guzowski).

Finally, Sandia's General and Administrative charges and Technology Tax charges amount to $13K.

Therefore, The total charges to Task 1 should be $78K. The budget report shows total charges of $88K; however, as mentioned above, once the one-manth charged by mistake against this task is corrected, the net charges should be reduced by about $10K.

FIN A1165, Task I - Licensing Methodology Assistance
Subcase 1183.010
February 1988

THIS IS AN ESTIMATE ONLY AND MAY NOT MATCH THE INVOICES SENT TO NRC BY SANDIA'S ACCOUNTING DEPARTMENT.

	Current Month	Year -to- Date
I. Direct Manpower (man-months of charged effort)	5.0	7.1
II. Direct Loaded Labor Costs	43	62
Materials and Services	0	2
ADP Support (computer)	0	0
Subcontracts	2	13
Travel	1	2
G&A	5	8
Other (computer roundoff)	-1	-1
TOTAL COSTS	50*	88

III. Funding Status

Prior FY Carryover	FY 88 Projected Funding Level	FY 88 Funds Received to Date	FY 88 Funding Balance Needed
$68K	$248K	$180K	None

*Includes $10K of staff-time charges by mistake: will be corrected

PROGRAM:	Identification and Analysis of Uncertainties		FIN A1165 Task II
CONTRACTOR:	Sandia National Laboratories	BUDGET PERIOD:	10/87 - 9/88
NMSS PROGRAM MANAGER:	D. Galson	BUDGET AMOUNT:	$495K
CONTRACT PROGRAM MANAGER:	R. M. Cranwell	FTS PHONE:	844-8368
PRINCIPAL INVESTIGATORS:	E. J. Bonano P. A. Davis	FTS PHONE: FTS PHONE:	844-5303 846-5421

PROJECT OBJECTIVE

To identify, analyze, and recommend generic methodologies for treating uncertainties associated with performance assessments of HLW repositories.

ACTIVITIES DURING FEBRUARY 1988

Subtask 2.1

I. Recommended techniques for assessing compliance with the EPA's HLW repository containment requirement (40CFR191.13)

No activity.

Subtask 2.2

I. Identification, evaluation, quantification, and reduction of uncertainty in HLW repository performance assessments: a preliminary report.

NRC written comments on the scoping document submitted last fiscal year are yet to be received.

Subtask 2.3

I. Elicitation and use of expert judgement in dealing with uncertainty in HLW repository performance assessments.

Some meetings have been held with potential consultants that will assist Sandia in the preparation of this report.

Subtask 2.4

I. Methods for analyzing uncertainty in HLW repository performance assessment models.

No activity.

II. Approaches to building confidence in HLW repository performance assessment models.

No activity.

Subtask 2.5

I. Methodology for scenario development and screening.

No activity this month; however, with the exception of incorporating a section on the use of expert judgement, this report is nearly complete.

II. Recommended methodologies for the analysis of data and parameter uncertainty in HLW repository performance assessment.

An extensive search of the scientific literature has been carried out to identify studies related to the development and application of uncertainty and sensitivity analysis techniques. This search has produced between 400-500 articles, reports, and books in this area. Currently, a review of this material is ongoing. The material has been classified into five major categories: (1) error propagation, (2) Monte Carlo techniques, (3) response surface methodology, (4) Fourier amplitude sensitivity test, and (5) differential analysis (including adjoint and Green's function techniques). Several computer codes that implement various of these techniques have been identified. About 12-15 review and comparison studies involving some of these techniques for uncertainty and sensitivity analyses have been found. The literature search is still ongoing; however, the majority of this effort is now complete.

Currently, the major effort is in reading, organizing, and assimilating the literature described above. Some writing has started. A brief chapter on error propagation has already been written which may undergo revision as the rest of the report progresses. The major writing effort at present involves differential analysis with emphasis on adjoint techniques. This is so because, even though many talk about adjoint methods, few really understand both conceptually and computationally the technique.

II. The use of expert judgement to estimate data and parameter uncertainty.

No activity.

III. Identification, analysis, quantification, and reduction of data and parameter uncertainty in HLW repository performance assessment.

No activity.

FIN A1165, Task II - Identification and Analysis of Uncertainties
Subcase 1183.020
February 1988

THIS IS AN ESTIMATE ONLY AND MAY NOT MATCH THE INVOICES SENT TO NRC BY SANDIA'S ACCOUNTING DEPARTMENT.

	Current Month	Year-to-Date
I. Direct Manpower (man-months of charged effort)	.1	2.3 P
II. Direct Loaded Labor Costs	2	27
Materials and Services	0	1
ADP Support (computer)	0	0
Subcontracts	0	13
Travel	0	5
G&A	0	5
Other (computer roundoff)	0	0
TOTAL COSTS	2	51

III. Funding Status

Prior FY Carryover	FY 88 Projected Funding Level	FY 88 Funds Received to Date	FY 88 Funding Balance Needed
$60K	$495K	$435K	None

PROGRAM:	Probability Techniques		FIN A1165 Task III
CONTRACTOR:	Sandia National Laboratories	BUDGET PERIOD:	10/87 - 9/88
NMSS PROGRAM MANAGER:	D. Galson	BUDGET AMOUNT:	$240K
CONTRACT PROGRAM MANAGER:	R. M. Cranwell	FTS PHONE:	844-8368
PRINCIPAL INVESTIGATORS:	E. J. Bonano	FTS PHONE:	844-5303
	P. A. Davis	FTS PHONE:	846-5421

PROJECT OBJECTIVE

To identify techniques for assigning probabilities to geologic processes and events.

ACTIVITIES DURING FEBRUARY 1988

Subtask 3.1

I. Techniques for estimating probabilities of events and processes affecting the performance of geologic repositories: a literature review.

No activity this month.

Subtask 3.2

I. Recommended techniques for estimating probabilities of events and processes affecting the performance of geologic repositories: assessing compliance with the EPA's containment requirements (40CFR191.13).

No activity this month.

FIN A1165, Task III - Probability Techniques
Subcase 1183.030
February 1988

THIS IS AN ESTIMATE ONLY AND MAY NOT MATCH THE INVOICES SENT TO NRC BY SANDIA'S ACCOUNTING DEPARTMENT.

		Current Month	Year -to- Date
I.	Direct Manpower (man-months of charged effort)	0.1	0.7
II.	Direct Loaded Labor Costs	1	8
	Materials and Services	0	0
	ADP Support (computer)	0	0
	Subcontracts	0	10
	Travel	0	0
	G&A	0	2
	Other (computer roundoff)	1	0
	TOTAL COSTS	2*	20

III. Funding Status

Prior FY Carryover	FY 88 Projected Funding Level	FY 88 Funds Received to Date	FY 88 Funding Balance Needed
$120K	$190K	$70K	None

*Admistrative charges.

PROGRAM:	Maintenance and Management of PA Codes		FIN A1165 Task IV
CONTRACTOR:	Sandia National Laboratories	BUDGET PERIOD:	10/87 - 9/88
NMSS PROGRAM MANAGER:	D. Galson	BUDGET AMOUNT:	$50K
CONTRACT PROGRAM MANAGER:	R. M. Cranwell	FTS PHONE:	844-8368
PRINCIPAL INVESTIGATORS:	E. J. Bonano	FTS PHONE:	844-5303
	P. A. Davis	FTS PJONE:	846-5421

PROJECT OBJECTIVE

To provide for a program of computer code maintenance and configuration management for codes developed for the NRC's HLW performance assessment program.

ACTIVITIES DURING FEBRUARY 1988

Subtask 4.5

Reports on performance assessment computer code maintenance and QA.

No activity.

Management Issues

The NMSS PM in his response to the monthly progress report for January informed Sandia that all but $5K of the funds allocated for this task shall be moved to Task 5 to cover the expenditures associated with the preparation of the SCP Review Guides. As a result, the work planned for this task will not be performed. Several activities initated under FIN A1158 were scheduled to be completed under this task. Sandia will summarize these activities in writing and forward the summary to the NMSS PM.

The funds have not been moved to Task 5 yet because Sandia was informed by Neil Coleman (NMSS PM for FIN A1158) that all costs incurred under A1158 during February pertaining to Code Maintenance should be moved to Task 4 under A1165. There seems to be a discrepancy on the instructions Sandia is receiving from the NMSS PMs for A1158 and A1165. This discrepancy must be resolved at NRC and Sandia notified in writing of its resolution before funds can be moved to Task 5.

FIN A1165, Task IV - Maintenance and Management of PA Codes
Subcase 1183.040
February 1988

THIS IS AN ESTIMATE ONLY AND MAY NOT MATCH THE INVOICES SENT TO NRC BY SANDIA'S ACCOUNTING DEPARTMENT.

	Current Month	Year -to- Date
I. Direct Manpower (man-months of charged effort)	0	0
II. Direct Loaded Labor Costs	0	0
Materials and Services	0	0
ADP Support (computer)	0	0
Subcontracts	0	0
Travel	0	0
G&A	0	0
Other (computer roundoff)	0	0
TOTAL COSTS	0	0

III. Funding Status

Prior FY Carryover	FY 88 Projected Funding Level	FY 88 Funds Received to Date	FY 88 Funding Balance Needed
None	$50K	$50K	None

PROGRAM:	Technical Assistance for SCP Review	FIN A1165 Task V
CONTRACTOR:	Sandia National Laboratories	BUDGET PERIOD: 10/87 - 9/88
NMSS PROGRAM MANAGER:	D. Galson	BUDGET AMOUNT: $45K
CONTRACT PROGRAM MANAGER:	R. M. Cranwell	FTS PHONE: 844-8368
PRINCIPAL INVESTIGATORS:	E. J. Bonano P. A. Davis	FTS PHONE: 844-5303 FTS PHONE: 846-5421

PROJECT OBJECTIVE

To develop internal staff guidance for review of the draft consultation SCP's and final SCP's in the area of performance assessment, to review selected parts of the draft and final SCP's, and to review NRC staff comments on selected parts of the draft and final SCP's.

ACTIVITIES DURING FEBRUARY 1988

No activity this month.

FIN A1165, Task V - Technical Assistance for SCP Review
Subcase 1183.050
February 1988

THIS IS AN ESTIMATE ONLY AND MAY NOT MATCH THE INVOICES SENT TO NRC BY SANDIA'S ACCOUNTING DEPARTMENT.

		Current Month	Year -to- Date
I.	Direct Manpower (man-months of charged effort)	0.2	3.6
II.	Direct Loaded Labor Costs	2	33
	Materials and Services	0	0
	ADP Support (computer)	0	0
	Subcontracts	6	39
	Travel	1	2
	G&A	1	8
	Other (computer roundoff)	-1	-1
	TOTAL COSTS	9*	81

III. Funding Status

Prior FY Carryover	FY 88 Projected Funding Level	FY 88 Funds Received to Date	FY 88 Funding Balance Needed
None	$45K	$45K	$None

*Includes admistrative charges and contractor charges for December 1987 and January 1988.

PROGRAM:	Short-Term Technical Assistance		FIN A1165 Task VI
CONTRACTOR:	Sandia National Laboratories	BUDGET PERIOD:	10/87 - 9/88
NMSS PROGRAM MANAGER:	D. Galson	BUDGET AMOUNT:	$64K
CONTRACT PROGRAM MANAGER:	R. M. Cranwell	FTS PHONE:	844-8368
PRINCIPAL INVESTIGATORS:	E. J. Bonano	FTS PHONE:	844-5303
	P. A. Davis	FTS PHONE:	846-5421

PROGRAM OBJECTIVE

To provide, on short notice, general technical assistance on HLW matters related to Tasks 1 through 5 that would not be provided in the normal course of the work in these tasks.

ACTIVITIES DURING FEBRUARY 1988

No activities.

FIN A1165, Task VI - Short Term Technical Assistance
Subcase 1183.060
February 1988

THIS IS AN ESTIMATE ONLY AND MAY NOT MATCH THE INVOICES SENT TO NRC B SANDIA'S ACCOUNTING DEPARTMENT.

	Current Month	Year -to- Date
I. Direct Manpower (man-months of charged effort)	0.0	0.0
II. Direct Loaded Labor Costs	0	0
Materials and Services	0	0
ADP Support (computer)	0	0
Subcontracts	0	0
Travel	0	1
G&A	0	0
Other (computer roundoff)	0	0
TOTAL COSTS	0	1*

III. Funding Status

Prior FY Carryover	FY 88 Projected Funding Level	FY 88 Funds Received to Date	FY 88 Funding Balance Needed
$19K	$39K	$20K	None

*Still attempting to find where this charge came from.

FIN A1165
Total for Case 1183.000
February 1988

THIS IS AN ESTIMATE ONLY AND MAY NOT MATCH THE INVOICES SENT TO NRC BY SANDIA'S ACCOUNTING DEPARTMENT.

	Current Month	Year -to- Date
I. Direct Manpower (man-months of charged effort)	5.4	12.7
II. Direct Loaded Labor Costs	48	130
Materials and Services	0	3
ADP Support (computer)	0	0
Subcontracts	8	75
Travel	2	9
G&A	6	23
Other (computer roundoff)	-1	1
TOTAL COSTS	63*	241

III. Funding Status

Prior FY Carryover	FY 88 Projected Funding Level	FY 88 Funds Received to Date	FY 88 Funding Balance Needed
$267K	$1067K	$800K	None

*Includes $10K of staff-time charges by error; will be corrected.

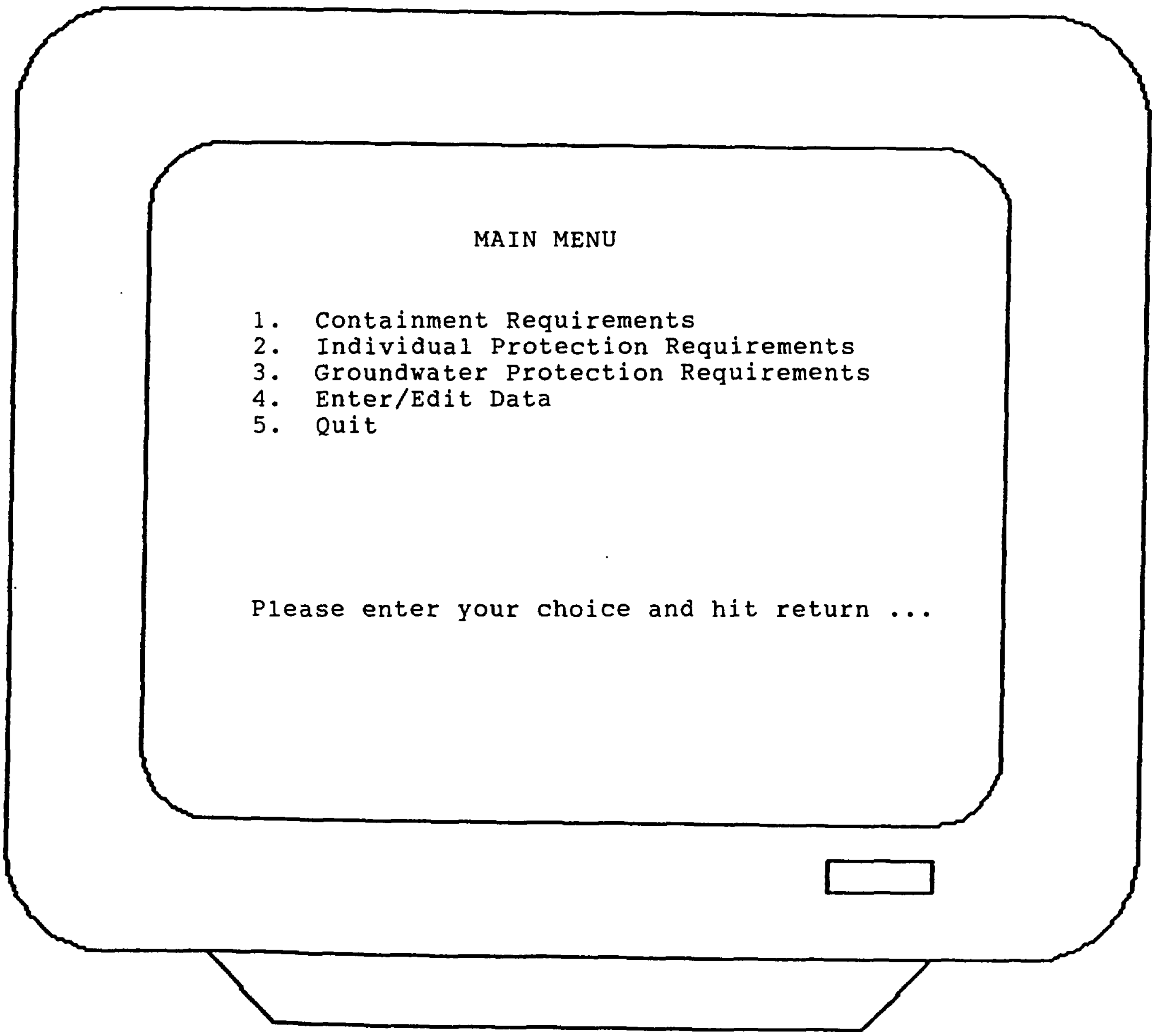

Figure 2. Sample LAMTRAX Main Menu

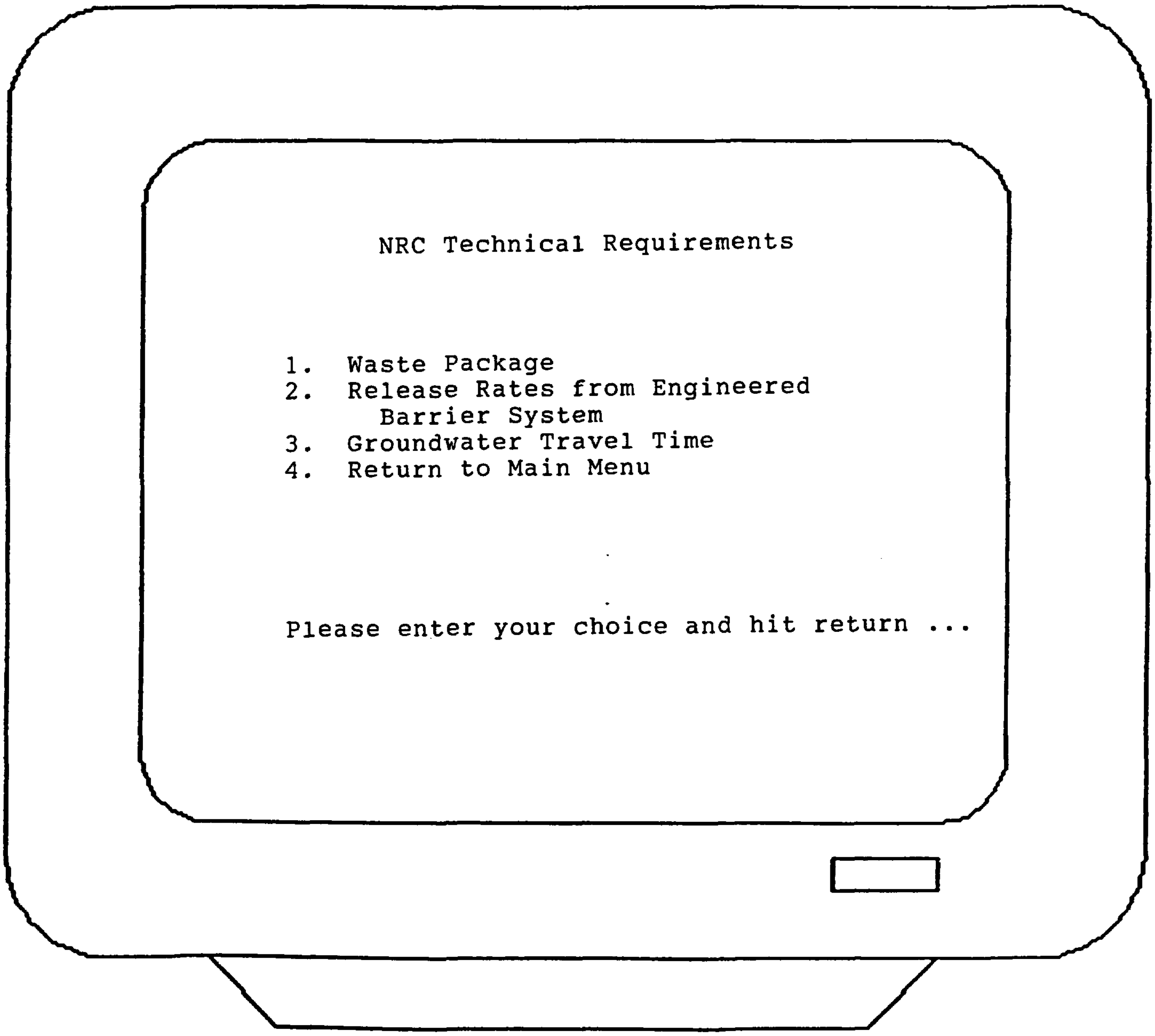

Figure 3. Sample LAMTRAX Technical Requirements Menu

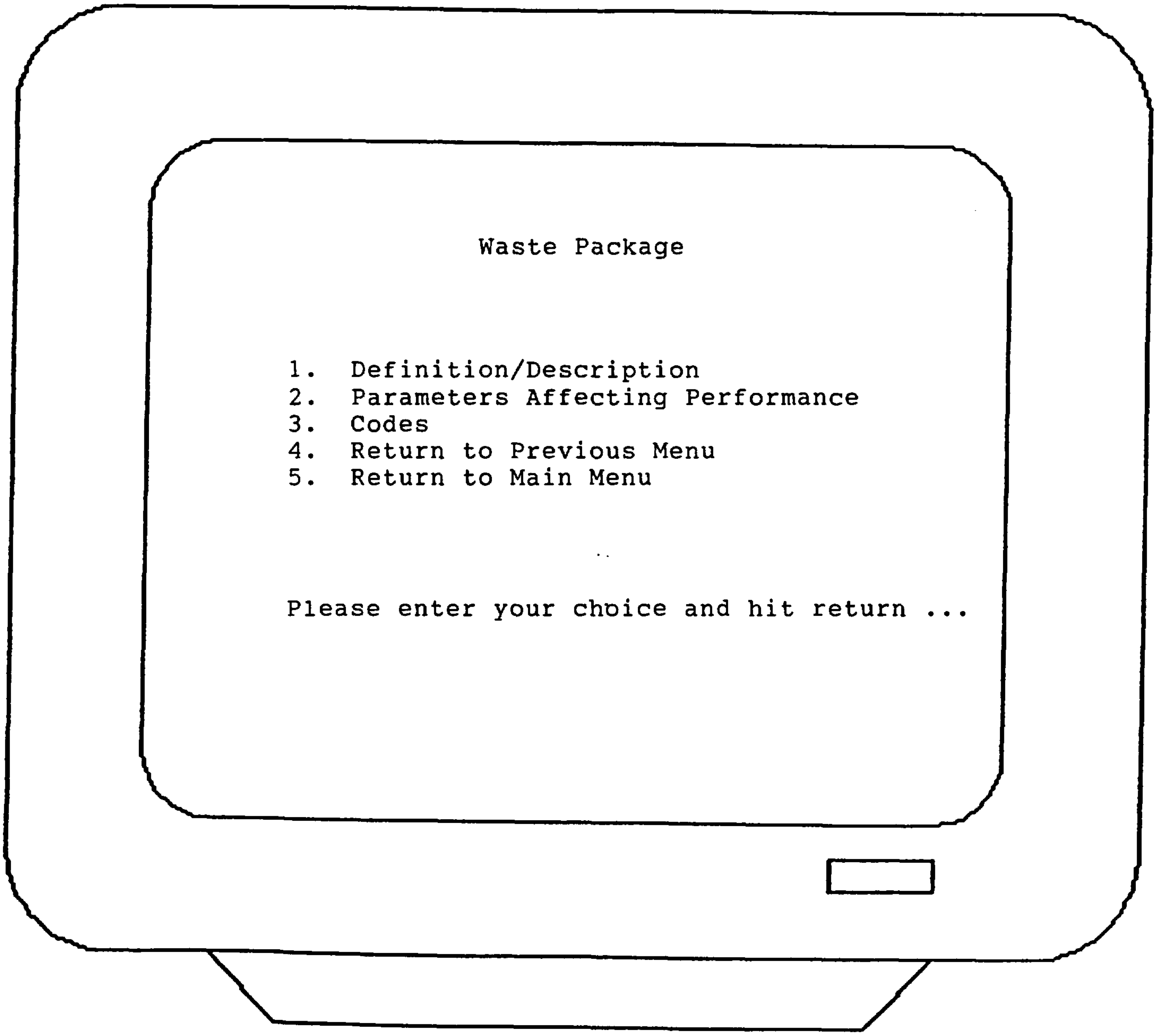

Figure 4. Sample LAMTRAX Waste Package Menu

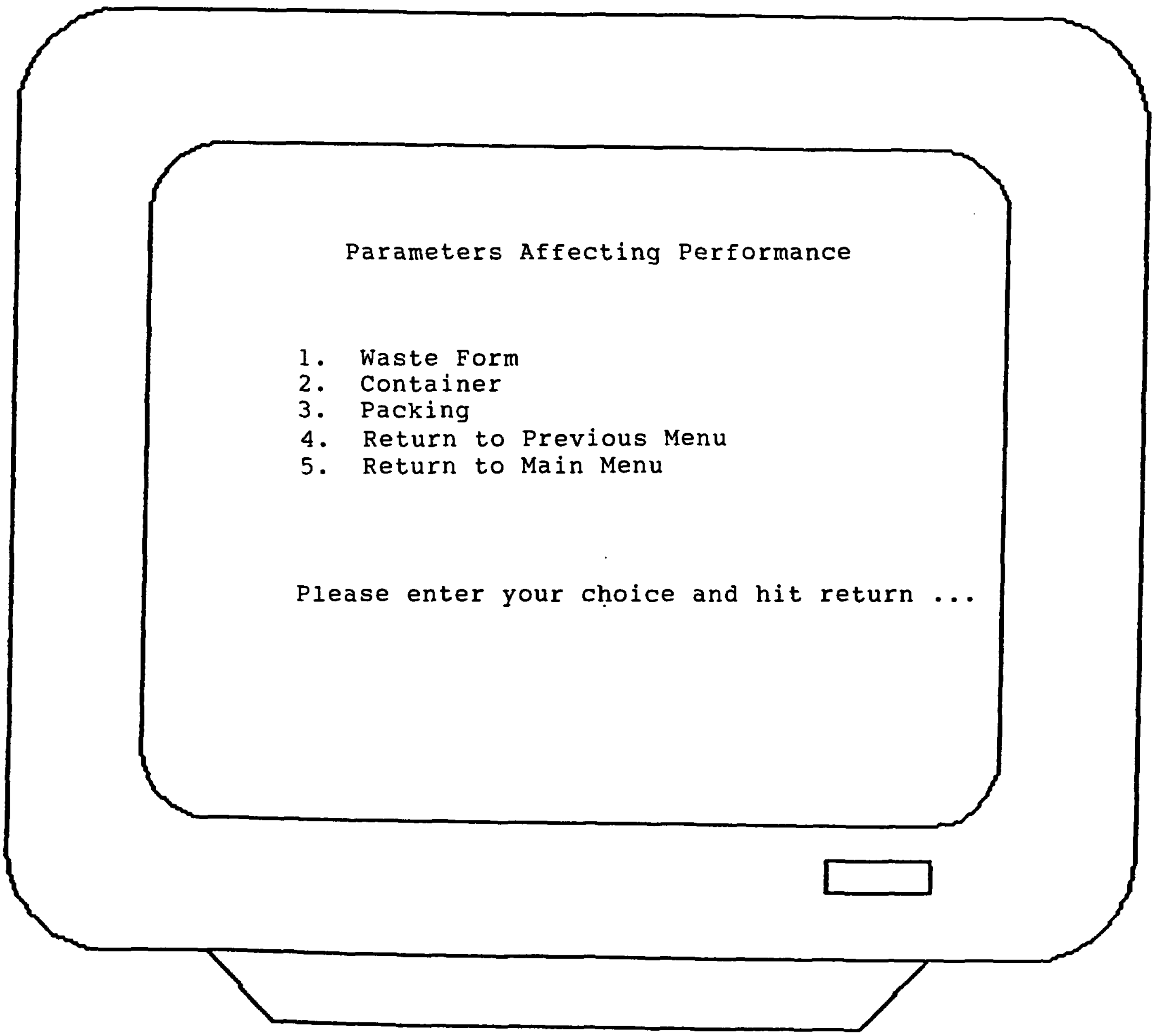

Figure 5. Sample LAMTRAX Parameters Menu

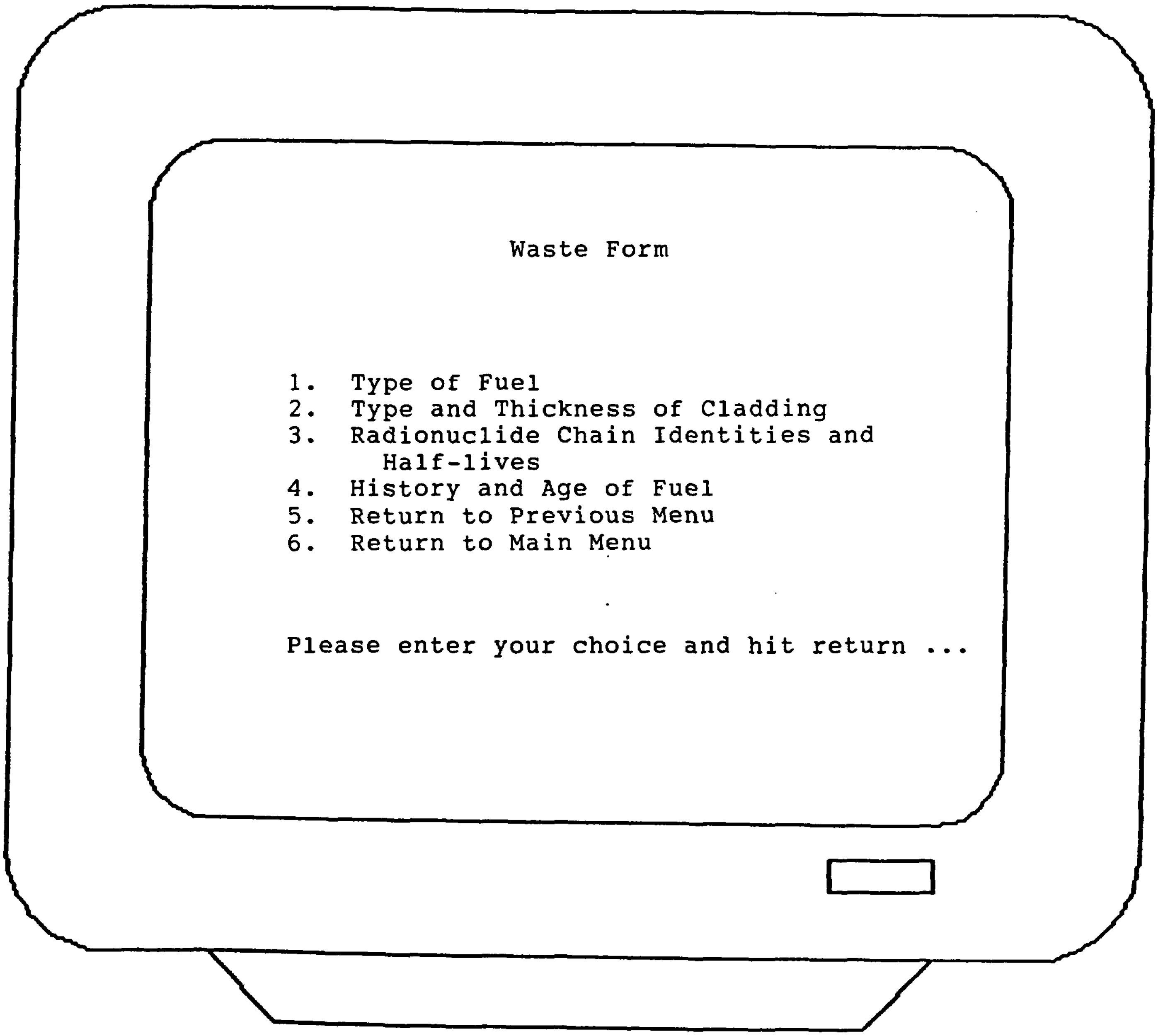

Figure 6. Sample LAMTRAX Waste Form Menu

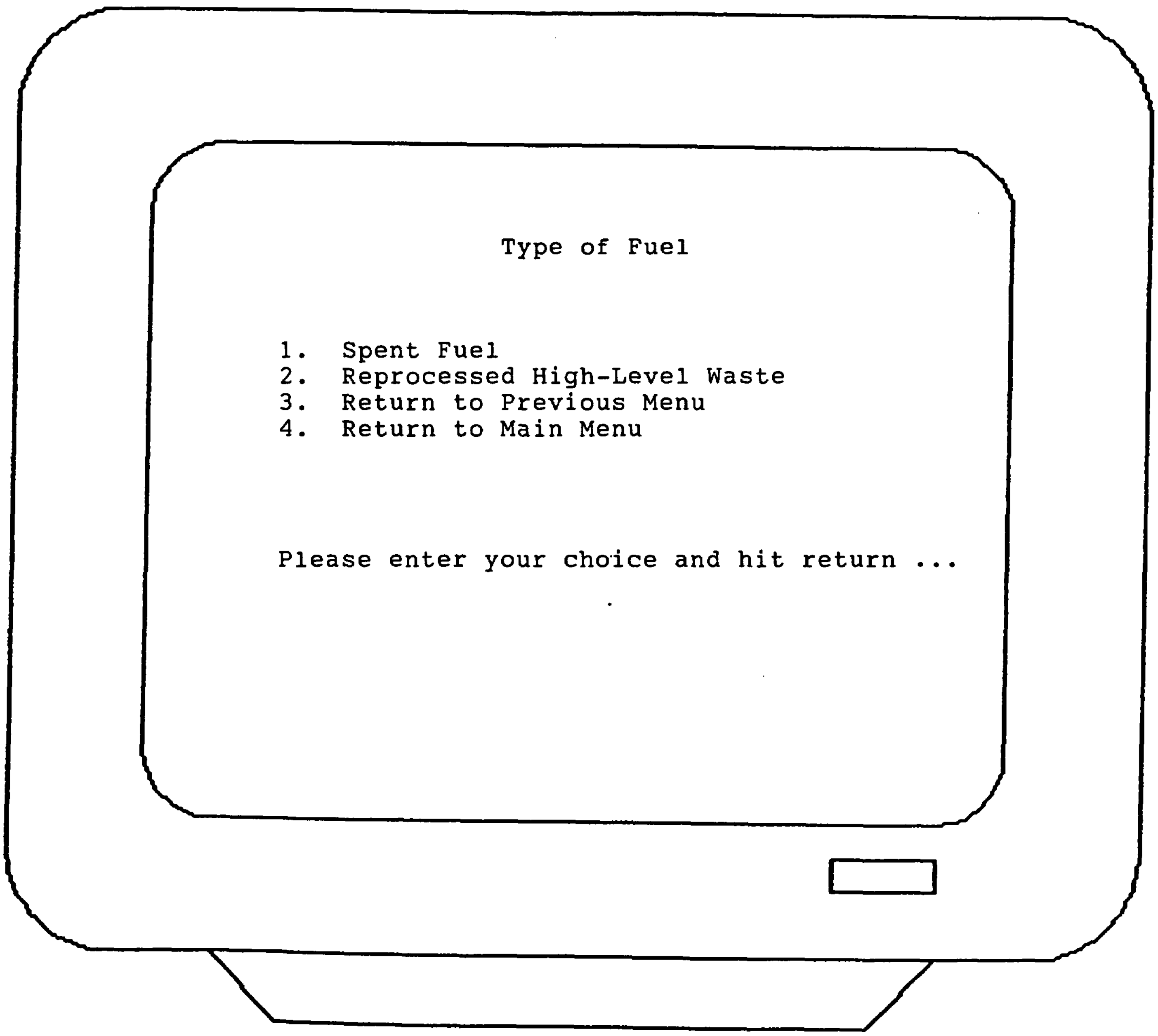

Figure 7. Sample LAMTRAX Fuel Type Menu

Identification of Parameters Used in Models and Codes

Preliminary Draft of Task 1.1.C
Overall Licensing Assessment Project

March 4, 1988

M.T. Goodrich

Identification of Parameters Used in Models and Codes

The purpose of this section of the report was to identify the parameters used in the codes and models needed in the methodology. This process is complicated by the fact that performance assessment techniques have never been applied in a consistent manner using validated codes. Moreover, there appears to be some confusion over the use of the words "code" and "model". For the purpose of this report, a "code" is a computer program that was written to use numerical techniques to solve a mathematical expression. For example, SWIFT II and NEFTRAN are codes. A model, however, is a conceptualization of a physical system; it may or may not include assumptions about the system that make it easier and less expensive to run the code. It is beyond the scope of this study to list all the parameters of all the codes that might be used in licensing assessment. This is because most models do not use all the input variables available for a code. For example, SWIFT II has nearly 300 possible variables for input; most models use less than half that many (Reeves et al., 1986c). Therefore the main emphasis of this section is models. If one requires a complete list of all possible input variables to a code, references are given so the interested reader may refer to the appropriate documentation.

Table 1 outlines some parameters that may be significant with regard to performance assessment modelling. When actual models are identified, the parameters and the appropriate value will be specified. Section 3.0 of the outline in Table 1 deals directly with codes. Given the fact that, at this time, no all-inclusive list of validated performance assessment codes has been published, only an initial sampling of available codes is presented here (Table 2).

Table 1. Sample Outline for Identification of Parameters Used in Models and Codes.

1.0 Introduction

2.0 Models

2.1 Model 1
2.1.1 Description of Model
2.1.2 References
2.1.3 Parameters (in no particular order)
2.1.3.1 Aquifer Properties
2.1.3.1.1 Hydraulic Conductivity
2.1.3.1.2 Porosity (porous media and fracture)
2.1.3.1.3 Hydraulic Gradient
2.1.3.1.4 Dispersivity
2.2.3.1.5 Molecular Diffusion
2.2.3.2...
2.1.3.2 Native Fluid Properties
2.1.3.2.1 Density
2.1.3.2.2 Viscosity
2.1.3.2....
2.1.3.3 Secondary (Contaminant) Fluid Properties
2.1.3.3.1 Density
2.1.3.3.2 Viscosity
2.1.3.3...
2.1.3.4 Solid Rock Properties
2.1.3.4.1 Overburden Density
2.1.3.4.2 Compressibility
2.1.3.4.3 Fractures
2.2.3.4.3.1 Location
2.2.3.4.3.2 Orientation
2.2.3.4.3.3 Aperture
2.2.3.4.4 Mechanical Properties
2.2.3.4.4.1 Compressive Strength
2.2.3.4.4.2 Transient Behavior (e.g., creep)
2.1.3.5 Grid Discretization
2.1.3.5.1 Coordinate System
2.1.3.5.2 Number of x,y,z Nodes
2.1.3.5...
2.1.3.6 Boundary Conditions
2.1.3.6.1 Prescribed Head
2.1.3.6.2 Prescribed Flux
2.1.3.6...
2.1.3.7 Radionuclide Properties
2.1.3.7.1 Initial Concentration
2.1.3.7.2 Waste Form
2.1.3.7...
2.1.3.8. Sink/Source Data
2.1.3.8.1 Location of Sinks/Sources
2.1.3.8.1 Flux at those Locations
2.1.3.9 Time-Step Data
2.1.3.9.1 Steady state simulation
2.1.3.9.2 Transient state simuulation
2.1.3.10 Thermal Data

2.1.3.10.1 Depth v. Temperature
2.1.3.10.2 Viscosity v. Temperature
2.1.3.10.3 Rock Conductivity
2.1.3.10.4 Specfic Heat
2.1.3.10...
2.1.3.11 Geochemical Factors
2.1.3.11.1 Kd/Retardation
2.1.3.11.2 Eh, pH, etc.
2.1.3.11.3 Chemical Composition of Host Rock
2.1.3.11...
2.1.3.12 Waste Package Components
2.1.3.12.1 Waste Form
2.1.3.12.2 Container
2.1.3.12.3 Packing
2.1.3.12...

2.2 Model 2
.
.
.
2.i Model i

3.0 Codes

3.1 Code 1
3.1.1 Description of Code
3.1.2 List of Models Run on this Code
3.1.3 References for the Code and Models
3.2 Code 2
.
.
.
3.i Code i

Table 2. Partial List of Codes Available for Use in Performance Assessment.

Code	Function	Reference
CONVO	Probabilistic performance assessment of waste package.	Fuller, 1987
TACO2D	Thermal conduction of waste package.	Burns, 1982
JAC2D	Stress analysis of solids.	Thomas, 1982
TOUGH	Unsaturated groundwater flow.	Pruess and, Wang, 1984
NORIA	Unsaturated groundwater flow.	Bixler, 1985
USGS Modular	Saturated groundwater flow.	McDonald and Harbaugh, 1984
SWIFT II	Saturated groundwater flow, fracture flow, and radio-nuclide transport.	Reeves et al., 1986a & 1986b
NEFTRAN	Saturated groundwater flow and radionuclide transport.	Longsine et al., 1980
PABLM	Biosphere transport and dose-to-man.	Napier et al., 1980
AIRDOS	Atmospheric transport	Moore et al., 1979
LHS	Uncertainty analysis	Iman and Shorten-carier, 1984

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Potential Codes for Computing Groundwater Travel Time

FEMWATER Yeh and Ward, 1979.

This code was developed at Oak Ridge National Laboratory and uses the finite-element method to simulate saturated or unsaturated flow through porous media. A system may be modelled in the vertical or horizontal plane and can be anisotropic. In addition, non-linearities are dealt with by allowing the storativity and hydraulic conductivity to be functions of the pressure head. FEMWATER is two-dimensional and allows the user to simulate regions of saturated or unsaturated media. It also produces a continuous pressure distribution and velocity field. Assumptions implicit to the code are that 1) Darcy's Law is valid, 2) the hydraulic gradient is the only important driving force for flow, and 3) the non-linear soil properties and the hydraulic conductivity are functions of the pressure head only. The code was written in FORTRAN IV for use on an IBM 360 machine.

FE3DGW Gupta et al., 1979.

This three-dimensional finite-element code simulates saturated flow in a homogeneous or heterogeneous porous media and provides flow paths and groundwater travel times. It is considered a "far-field" code in the sense that it analyzes flow outside the disturbed zone. It can be used to model single or multiple layered systems with variable thicknesses in the geologic layers. Output consists of heads and velocity vectors; auxiliary programs may be available to plot node values, contour maps, and perform other output enhancing routines. Assumptions include that 1) Darcy's Law is valid, 2) the porosity and hydraulic conducttivity are constant with time, 3) gradients of fluid density, viscosity, and temperature do not affect the velocity field, and 4) the hydraulic conductivity principle axes are aligned parallel to the coordinate axes. The code is written in FORTRAN IV and was originally designed to run on a PDP-11/45 mini computer; by now it may also be compatable with larger machines. It has been used extensively in modelling groundwater flow in the Long Island, New York groundwater basin (Gupta and Pinder, 1978).

GWTT Sinnock, et al., 1986.

Generates probability distributions for groundwater travel times along flow paths. Uses a simplified Darcy's Law solution in both fractures and the matrix.

ISOQUOD Pinder, 1976.

This program computes flow in heterogenous, multi-dimensional, saturated media. Darcy's Law is applied with a transient leakage coefficient. The code contains both sink and source terms.

NORIA Bixler, 1985.

NORIA is designed to solve liquid, vapor, air, and energy transport in partially saturated and saturated porous media. The following mechanisms are included in NORIA: 1) transport of water, vapor, and air due to pressure gradients, 2) transport of water, vapor and air due to density gradients, 3) binary diffusion of vapor and air, 4) Knudsen diffusion of vapor and air, 5) thermo-diffusion of vapor and air, 6) conduction of sensible heat, 7) convection of sensible heat, 8) evaporation and condensation, 9) non-equilibrium and equilibrium vapor pressure model, and 10) capillary pressure. Nearly all the thermodynamic and constitutive properties in the model can be defined nonlinearly in terms of the remaining dependent or independent variables by the user. The code is written in FORTRAN and is operational on a CRAY machine.

SAGUARO Eaton et al., 1983.

SAGUARO solves Richard's Equation for flow through partially saturated porous media. It can deal with the effects of the capillary fringe and assumes a single-phase incompressible fluid. It also includes energy transport via conduction, convection, and dispersion.

SWIFT II Reeves et al., 1986.

SWIFT is a fully transient three-dimensional finite-difference code that solves the coupled equations for flow and transport in porous or fractured media. When the dual-porosity option is activated, one set of equations is solved for the fracture and one for the matrix. The equations are the same except for the sink/source terms representing exchange processes with the matrix. It can also simulate heat transport and brine migration. Additionally, the model grid can be discretized in either cartesian or cylindrical coordinates. Other applications include radionuclide transport from a geologic repository, and salt-water intrusion, injection of industrial wastes, heat storage, salt dissolution. It is currently being used in the Department of Energy's performance assessment at the Waste Isolation Pilot Plant (WIPP) in southeastern New Mexico. It was written in FORTRAN V and is currently operational on CDC and CRAY machines.

TOUGH Pruess and Wang, 1984.

TOUGH solves the two-phase flow of air and water in vapor and liquid phases and heat flow in a fully coupled way. The formulation used in TOUGH is analogous to that used in multiphase, multicomponent geothermal or steam-flooded hydrocarbon reservoirs. The governing fluid flow equations account for gaseous diffusion, Darcy flow, capillary pressure, vaporization and condensation. Vaporization and condensation with latent heat effects and conduction and convection of heat flow are included in the energy equation. Water, air, and rock are assumed to be in thermodynamic equilibrium at all times. The flow domain can include liquid, gas, and two-phase regions, indicating that the code handles both saturated or unsaturated flow problems either individually or simultaneously. The thermophysical properties of liquid and vaporized water are represented by the International Formulation Committee's steam tables. Air is approximated as an ideal gas and adjectivally of partial pressures is assumed for air-vapor mixtures. TOUGH solves three nonlinear partial differential equations simultaneously. These consist of the conservation equations for air, water, and heat. Air and water can be transported in either the liquid or gas phases. The dissolution of air in water is represented by Henry's law. Flow is governed by Darcy's law. The code can simulate flow in one, two, or three dimensions because the method of solution is based on a very general integrated finite-difference method. It is written FORTRAN and is operational on CRAY and CDC machines.

UNSAT2 Neuman et al., 1974

UNSAT2 is a well-known finite-element code that was developed to simulate non-steady flow in partially-saturated media. It is two-dimensional and can model flow in the vertical or horizontal plane. It has the capability to treat a variety of boundary conditions including prescribed pressure head, prescribed flux, recharge boundaries, and seepage faces. It is also capable of describing water uptake by plant roots and flow to partially or fully penetrating wells. Important assumptions by the authors are that 1) Darcy's Law is valid, 2) the hydraulic gradient is the only important mechanism for driving flow, 3) the maximum rate of transpiration is determined by atmospheric conditions, and 4) the hydraulic conductivity at each node is expressed as a symmetric tensor. The code was written in FORTRAN IV for an IBM 370/165 machine.

USGS Modular McDonald and Harbaugh, 1984.

The Modular code is an outgrowth of the USGS2D and USGS3D codes. It uses a block-centered finite-difference approach to solve two- or three-dimensional problems. It is a very popular code that allows for the simulation of wells, recharge, rivers, evapotranspiration, and sub-surface drains. It allows for no-flow boundaries along the outside of the grid (if desired) and constant head boundaries at other nodes. It was designed for modelling saturated flow in porous media and does allow for anisotropy. It was written in FORTRAN IV and has been run on IBM, CDC, Prime, DEC, and CRAY machines.

VTT Reisenauer, 1979.

This code is designed for steady or non-steady flow in multilayered porous media. The system may be confined, semi-confined, or unconfined. Two-dimensional flow in horizontal layers is simulated using finite-difference methods for saturated media. A 2-D system may be transformed to a quasi-3-D system by a potential-driven leakage term. Output includes velocities, flowpaths, and travel times in the form of plots and numerical listings. Some important assumptions are that 1) the free-surface slope and aquifer bottom slope are minimal ($< 5^{\circ}$), 2) vertical velocities are small and can be neglected, 3) the capillary fringe is ignored, and 4) seepage faces are ignored. The code was written in FORTRAN IV and is supposed to be operational on a CDC machine.

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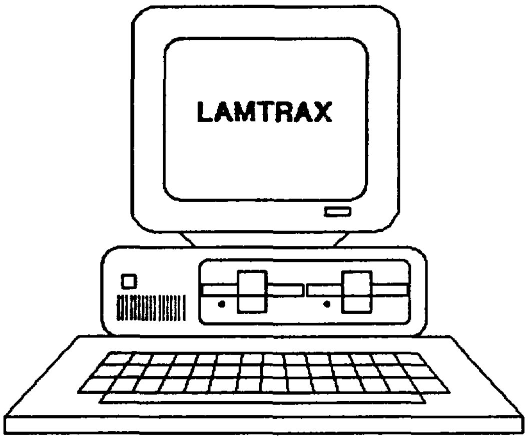
LICENSING ASSESSMENT METHODOLOGY TRACKING SYSTEM



Preliminary Draft of Task 1.1.D
Overall Licensing Assessment Project
March 4, 1988

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Licensing Assessment Methodology Tracking System

This section of the report deals with the development and implementation of a tracking scheme for monitoring the status of codes and parameters essential to the licensing assessment methodology. The licensing assessment methodology tracking system (LAMTRAX) is a user-friendly database designed to allow the technician to review data needs, areas needing further development, and parameter uncertainty associated with the methodology. In Section 1.0, the structure and design of the system is discussed. In Section 2.0, the actual implementation procedures are reviewed.

Section 1.0 LAMTRAX Organizational Structure

The tracking scheme is well suited for a hierarchal organization. Figure 1 is a flow chart that depicts the overall design of LAMTRAX. This figure gives only a basic overview of the structure; a complete outline of the system as it currently exists is listed in Table 1. Basically, the system is designed around the three EPA System Requirements (containment requirements, individual protection requirements, and groundwater protection requirements) with an increasing degree of complexity at each level of the structure. When the system is operational, the user will be able to easily review all of the different components of the methodology or to go to directly to a given area of interest.

Section 2.0 LAMTRAX Implementation

This section of the report proposes how the tracking system for the Licensing Assessment Methodology (LAM) will be implemented. The system design described in Section 1.0 is very hierarchical in its structure. This tree structure lends itself well to an interactive menu-driven environment for retrieval of information. Sandia has developed LAMTRAX and proposes to implement it on an IBM PC/AT or compatible environment using dBASE III Plus* (Version 1.1) as the database management system. This version is not a copy protected version of dBASE III where earlier versions are. The ability to install dBASE III Plus on a hard disk with no copy protection permits start-up without first having to insert the master disk. In addition, back-up of all system software is made possible.

Although dBASE III Plus is a relational (two-dimensional table) database management system, the tree-structured nature of the information can be achieved by multiple databases linked together. dBASE III Plus is a proprietary software package that is acceptable to the NRC/Office of Resource Management and contains the query language and programming features of its command language that allow an interactive, user-friendly, menu-driven system to be developed. Figures 2-7 give examples of the kind of information a user might expect to see on the screen when they access LAMTRAX. Since it was impossible to show the entire tracking system in this manner, one branch of the structure was chosen for an example. In this case, structure given is: Main Menu -> Containment Requirements -> Waste Package -> Parameters Affecting Performance -> Waste Form -> Type of Fuel. Again, for a complete description of the system, the reader is referred to Table 1. Screen forms will be developed to allow editing of the existing information contained in the system when necessary. Retrieval of components, parameters, computer codes, and other information that are part of the LAM will be achieved through the use of nested menus and will require no knowledge of the structure of the database by the end user.

Documentation of the final LAMTRAX system will be provided in the form of a NUREG/CR. This document will provide the user with some history of the LAM, a reference to this report and other supporting material, some example query sessions, procedures for editing existing information if necessary, and instructions for initially installing LAMTRAX onto the user's computer from a diskette provided by Sandia. In addition, the structures of the individual databases will be described in case the need arises for future modifications. This installation diskette will contain all of the databases and the software developed by Sandia to drive the computerized system, but will not contain proprietary software such as DOS and dBASE III Plus.

When possible, other existing databases such as the Nuclear Energy Agency Data Bank will be investigated to provide guidance and data for the LAMTRAX system.

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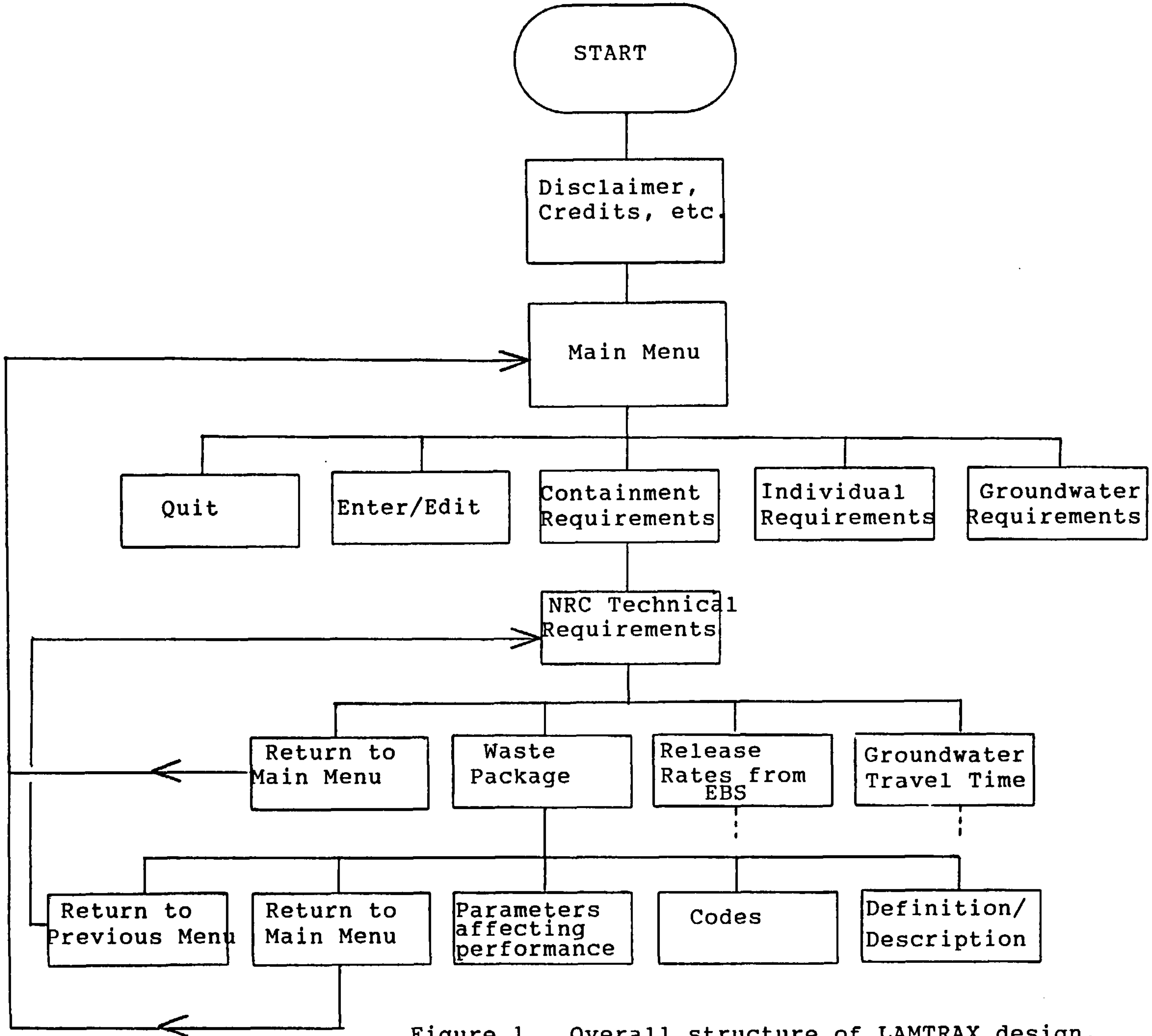

Figure 1. Overall structure of LAMTRAX design. Dashed lines under "Release Rates from EBS" and "Groundwater Travel Time" indicate that what follows is the same as for Waste Package.

Table 1. Outline of the Licensing Assessment Methodology Tracking System (LAMTRAX)

I. Banner
II. Credits
III. Disclaimer
IV. Description
V. of system
VI. Main Menu - EPA System Requirements

A. **Containment Requirements** (40CFR191.13)
1. Release limits apply to the accessible environment.
2. Release limits apply to first 10,000 years post closure.
3. Controlled Area shall not extend more than 5 km from edge of repository and shall not exceed 100 km^2.
4. Release limits computed in 40CFR191-Appendix A apply to release levels expected to occur with a cumulative probability of greater than 0.1 over the 10,000 year period.
5. Those same release limits, if increased by one order of magnitude, apply to release levels expected to occur with a cumulative probability of greater 0.001 over the 10,000 year period.
6. No limits are placed on release levels expected to occur with a cumulative probability of less than 0.001 over the 10,000 year period.

(A) NRC Technical Criterion

(1) Waste Package
a. Definition/description
1. "Waste Package" means the waste form and any containers, shielding, packing and other absorbent materials immediately surrounding an individual waste container (10CFR60.2).
b. Parameters affecting performance
1. Waste form
A. Type of fuel
1) Spent fuel
(a) BWR or PWR
1. Consolidated or unconsolidated
2) Reprocessed HLW
B. Type and thickness of cladding
C. Radionuclide chain identities and half-lives
D. History and age of fuel
2. Container
A. Mechanical/Structural integrity
1) Strength and elastic moduli
2) Fracture toughness
3) Thermal output
4) Failure modes

B. Corrosion properties
1) Uniform corrosion
2) Pitting
3) Intergranular Stress Corrosion Cracking (IGSCC)
4) Radiolysis
3. Packing
A. Type of material
B. Thickness
C. Sorbing properties
c. Codes
1. Code 1
A. Description of the code
B. Applicable models already run on the code
C. References
2. Code 2 ...
d. Return to previous menu
e. Return to main menu

(2) Release Rates from Engineered Barrier Systems
a. Definition/description
1. "Engineered Barrier System" means the waste package and the underground facility (10CFR60.2).
b. Parameters affecting performance
1. Transport through waste package (see "Waste Package")
2. Transport through Engineered Barrier System
A. Flow parameters
1) Boundary conditions
2) Other parameters (see "Groundwater Travel Time")
B. Coupled heat and mass transport
1) Heat source term
2) Thermal properties of waste package
(a) Density
(b) Conductivity
(c) Specific heat (heat capacity)
(d) Surface emittance
C. Transport through each layer of the waste package
1) Waste form (see "Waste Package")
2) Packing (see "Waste Package")
3) Backfill (see "Waste Package, Packing")
c. Codes (see "Waste Package")
d. Return to previous menu
e. Return to Main Menu

(3) Groundwater Travel Time
a. Definition/description
1. The travel time of a particle of water along the fastest path of likely radionuclide travel from the disturbed zone to the accessible environment. Minimum acceptable time is 1000 yrs (10CFR60.113).
b. Parameters affecting performance
1. Hydrologic factors
A. Hydraulic conductivity
B. Effective porosity

C. Hydraulic gradient
D. Fluid density
E. Dispersivity
F. Molecular diffusion
G. Other factors

2. Geologic factors
   A. Rock Type
   B. Degree of fracturing
      1) Orientation
      2) Location
      3) Aperture
      4) Porosity
   C. Thickness of formation

3. Geochemical factors
   A. pH
   B. Kd/retardation
   C. Chemical composition of host rock

4. Natural processes
   A. Volcanism
   B. Seismicity
   C. Subsidence
   D. Dissolution
   E. Flooding
   F. Glaciation
   G. Extreme erosion

5. Sensitivity/Uncertainty Analysis
   A. Spatial variation

6. Possible future rule changes

c. Codes (see "Waste Package")
d. Return to previous menu
e. Return to Main Menu

B. Individual Protection Requirements (40CFR191.15)

1. Apply to first 1000 years post-closure.
2. Annual shall be no more than 25 millirems to the whole body or 75 millirems to any organs.
3. This exposure limit assumes ingestion of 2 liters per day of water from a "significant source" of groundwater outside the controlled area.
4. A "significant source" is one that:
   (A) is saturated with water containing less than 10,000 mg per liter of total dissolved solids,
   (B) is within 2500 ft. (762 m) of the land surface.
   (C) has a transmissivity of at least 200 gallons per day per foot (2.9E-05 m^2/sec) provided that,
   (D) each of the undeground formations or parts of the underground formations included within the aquifer must have a hydraulic conductivity greater than 2 gallons per day per square foot (9.4E-07 m/sec), and
   (E) must be capbale of providing a sustained yield of 10,000 gallons per day (4.4E-04 m^3/sec) of water to a pumped or flowing well.

C. Groundwater Protection Requirements (40CFR191.16)
  1. Apply to first 1000 years post-closure
  2. Apply to Class I groundwaters that are:
     (A) within the controlled area or less than 5 km beyond the controlled area,
     (B) supplying drinking water for thousands of persons as of the date that the site is selected as a potential repository,
     (C) irreplacable in that no reasonable alternative source of drinking water is available.
  3. Radionuclide concentrations shall not exceed those established for community water systems in 40CFR141.

D. Enter/Edit data

E. Quit to DOS