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Review and Discussion of Code Linkage and Data Flow in Nuclear Waste Compliance Assessments

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Abstract

This report presents a review and discussion of data flow in a compliance assessment for high-level and transuranic waste, primarily the Containment Requirement of the Environmental Protection Agency (EPA) regulations, *40 CFR 191, Environmental Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level, and Transuranic Radioactive Wastes.* Two major points concerning data flow are presented. First, assuring the quality of a compliance assessment requires that the flow of data and linkage of computer codes be well defined and precisely controlled during execution. Second, the need to analyze many different scenarios using different computer codes requires a flexible data linkage. The manner of linking codes to simultaneously provide quality assurance and flexibility is emphasized, rather than specific computer codes used. Thus, this report is not a user's guide, but a description of how a compliance assessment system was implemented in accordance with EPA regulatory guidance. Although the methods described are general, all examples pertain to the Waste Isolation Pilot Plant project, which prompted development of the concepts.

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The file structure for the interface between computer programs, herein termed a computational data base, is based on the interface file used by the SNLA Engineering Analysis Department, whose foresight in establishing a simple but robust file structure is acknowledged.

Many individuals at SNLA have helped produce a workable procedure for assessing compliance with goals of the international Nuclear Energy Agency and regulations of the Environmental Protection Agency and Nuclear Regulatory Commission, upon which the executive package, CAMCON, is based. Although the review chapter on the SNLA procedure could not reference everyone, each individual's contribution is here acknowledged.

Contents

SUMMARY vii

NOMENCLATURE xi

1. INTRODUCTION 1

1.1 Purpose and Organization of Report 1
1.2 Objective of Code Linkage 1
Purpose 1
Need for Data Control 2
Scope of the Report 2
1.3 Relationship with Previous Performance Assessment Work 2
1.4 Evaluating Compliance with the EPA Standard 3
EPA Standard *(40 CFR 191)* 3
SNLA Compliance Evaluation 3
1.5 Methods Used to Perform Compliance Assessment 4
General Approach 4
Linking Codes and Controlling Data Flow 4
1.6 Background on WIPP 6
Purpose 6
Location 7
SNLA Role in Project 9
Influence of EPA Standard 10

2. ASSESSING COMPLIANCE OF DEEP GEOLOGIC REPOSITORIES 11

2.1 Risk Assessment in General 11
Background on Risk Assessment 11
Definitions 12
2.2 Regulatory Requirements for Geologic Repositories 13
EPA Regulations *(40 CFR 191)* 13
NRC Regulations *(10 CFR 60)* 19
2.3 Uncertainties in Compliance Evaluation 20
Sources of Uncertainty 20
Scenario Uncertainty 21
Model Uncertainty 22
Controlling Modeling Errors 23
Evaluating Modeling Uncertainty 25
Parameter Uncertainty 26
Controlling and Evaluating Parameter Uncertainty 26

3. SNLA COMPLIANCE ASSESSMENT METHODOLOGY 28

3.1 Tasks in Methodology 28
3.2 Task 1: Disposal System and Surrounding Area Characterization 30
System Components to Characterize 30
Iteration of Site Characterization 31
Important Information to Gather 31
3.3 Task 2: Scenario Development 32
3.4 Task 3: Consequence Modeling 33
Modeling Components 33
Component and Data Selection 36
3.5 Task 4: Sensitivity/Uncertainty Analysis 39
Uncertainty Analysis 39
Sensitivity Analysis 41
3.6 Task 5: Compliance Evaluation 43
Compliance with EPA Containment Requirements *40 CFR 191.13* 43
Compliance with Remaining EPA Requirements 46
Compliance with NRC Regulations 47
3.7 Benefits of Compliance Assessment 48

4. ADDITIONAL ASPECTS OF COMPLIANCE ASSESSMENTS 49

4.1 Multiple Passes in Compliance Assessment Procedure 49
4.2 Monte Carlo Sampling 52
4.3 Model Subdomains in Consequence Assessments 52
Regional Scale Model 53
Local Scale Model 53
Repository Scale Model 53
Setting Boundary Conditions 57
Interpolating from Coarse to Fine Grids 57
Interpolating from Fine to Coarse Grids 57
4.4 Requirements for CAMCON: Controller for Compliance Calculations 58

5. ASSURING ACCURATE DATA TRANSFER 61

5.1 Primary Data Bases 61
Requirements 61
Suggested Format 63
5.2 Secondary Data Bases 64
Development of a Secondary Data Base 64
Separate Files May Exist for Each Conceptual Model 64
General Features of a Secondary Data Base 64
5.3 Computational Data Base 65
Serial Linkage of Codes 65
Neutral File Linkage of Codes 66
General Features of Computational Data Base 69

6. CODE LINKAGE AND DATA FLOW 72

6.1 Mesh Generation Module 72
Purpose 72
Flow of Data 72
Tasks Performed 72
Support Module, Material Properties 74
Application to WIPP 74
6.2 Monte Carlo Sampling Module 74
Purpose 74
Flow of Data 74
Application to WIPP 75
6.3 Regional Fluid-Flow Module 78
Purpose 78
Support Module, ALGEBRA 78
Application to WIPP 78
6.4 Local Fluid-Flow Module 79
Purpose 79
Flow of Data 79
Interpolating between Model Scales 79
Application to WIPP 79
6.5 Repository/Shaft Module 81
Purpose 81
Flow of Data 81
6.6 Nuclide Transport Module 82
Purpose 82
Methods 82
Flow of Data 82
6.7 Plotting Module 84
6.8 Final Calculations 85
Containment Calculations 85
Groundwater Concentration and Dose Calculations 85
6.9 Summary of Data Flow 88

APPENDIX A: Computational Data Base, CAMDAT 90

APPENDIX B: Secondary Data Base 103

REFERENCES 109

Figures

1.1 Code linkage and data flow in nuclear waste compliance assessments 5

1.2 Location of the WIPP site in southeastern New Mexico 8

1.3 General stratigraphy at the WIPP site 9

1.4 Responsibilities of participants in the WIPP project 10

2.1 Containment and Assurance Requirements are the principal components of the EPA High-Level Waste Standard 14

2.2 Release limits of the Containment Requirements of the EPA Standard are probabilistically based 16

2.3 Many factors contribute to uncertainties in predictions; these factors must be controlled and evaluated 21

2.4 Modeling uncertainty originates from all three phases of model development 22

2.5 User errors, imperfect conceptual models, and imperfect mathematical models contribute to modeling uncertainty 24

2.6 Measurement errors, data reduction, and use of general data contribute to data uncertainty 27

3.1 SNLA's method for assessing repository compliance involves five tasks 29

3.2 Scenario development involves event and process identification, screening, scenario construction, and further screening 34

3.3 Four general criteria exist for screening scenarios 35

3.4 Six model categories were used in assessing the consequence of a scenario in the WIPP 37

3.5 Different stages of consequence calculations used to assess compliance with requirements of the HLW regulations 44

3.6 A complementary cumulative distribution function is produced for comparison with the EPA containment requirements 46

4.1 Better resource allocation occurs when iterating through the compliance assessment system in addition to iterating through the site characterization and facility design process 50

4.2 Simplified hypothetical network diagram showing interaction between compliance assessment methodology (scenario development and consequence modeling) and disposal system characterization (facility design and site and waste characterization) 51

4.3 Three model scales are typically used in compliance assessment 54

4.4 Repository modeling component must be assembled from four submodels 56

4.5 The WIPP will explore propagating information from a calibrated local model into the regional model by iterating boundary conditions at the interface between the local and regional hydrologic models 59

5.1 Analyst interprets data in primary data base to develop secondary data base 62

5.2 Serial coupling of codes is standard but not always ideal 66

5.3 Coupling through a computational data base ("neutral file") creates a modular structure 67

5.4 Order and types of data stored in a computational data base 70

5.5 Correspondence between generic computational data base and CAMDAT 71

6.1 Data flows from the secondary data base, to the mesh generator, and then into the computational data base 73

6.2 n_v-replications of the computational data base result from Monte Carlo sampling 76

6.3 Monte Carlo sampling can change material properties set by the material support module 77

6.4 Computational data base linked to a regional flow model through translators 78

6.5 Interpolation module sets local model boundary conditions 80

6.6 Source concentrations found from repository model after interpolating boundary conditions from local model 81

6.7 Transport calculations made using repository and local model information 83

6.8 Results can be displayed throughout computations when using computational data base 84

6.9 The final task combines release results from $n_s \bullet n_v$ runs to generate a CCDF for comparison with EPA Standard *(40 CFR 191.13)* 86

6.10 Biosphere transport module used with undisturbed scenario to assess compliance with individual protection requirement *(40 CFR 191.15)* 87

6.11 Data flow in consequence assessments is complex; careful data control is necessary 89

A.1 Storage of WIPP finite-difference mesh in CAMDAT 90

A.2 Correspondence between generic computational data base and CAMDAT 97

B.1 The secondary data base consists of two separate file groups 103

Table

2.1 Cumulative release limits, L_i, to the accessible environment 10,000 yr after disposal *(40 CFR 191, Appendix A)* 16

Summary

EPA Requirements

Geologic repositories for high-level waste (HLW), spent fuel, and transuranic (TRU) waste must demonstrate compliance with requirements specified in regulations of the Environmental Protection Agency (EPA). The EPA Standard, *Environmental Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level, and Transuranic Radioactive Wastes, (40 CFR 191),* is divided into two parts. Subpart A sets limits on annual radiation doses to the public during operation of the facility. Although currently vacated by federal courts (and thus may change), Subpart B had set post-closure limits for:

- Total cumulative release of radionuclides into the accessible environment for 10,000 years (Containment Requirements)
- Annual radiation doses to the public for 1000 years (Individual Protection Requirements)
- Contamination of special sources of groundwater for 1000 years (Groundwater Protection Requirements).

Five Tasks of Compliance Assessment

Assessing compliance with the cumulative release limits for 10,000 years (i.e., the Containment Requirement) requires extensive calculations that, in turn, require a well-defined procedure. Similar to other risk assessments, this procedure usually consists of five tasks:

- Collecting data on waste properties, site and regional geology and hydrology, and facility design to characterize the disposal system (regional and disposal-system characterization)
- Identifying the events and processes whereby radionuclides might be released (scenario development)
- Predicting the amount of these releases through modeling (consequence analysis)
- Evaluating the uncertainties associated with these predictions and the most important variables influencing these uncertainties (sensitivity/uncertainty analysis)
- Comparing the predicted releases with government regulations (compliance evaluation).

The first two tasks establish the conceptual model(s) of the disposal system and surrounding region for each significant scenario. The third task mathematically simulates the conceptual model, usually by a system of computer codes, each using different solution methods and subdomains of the disposal system that must be linked together.

The fourth task requires that uncertainties be propagated through the analysis and that important parameters influencing these uncertainties be identified. The identification of important parameters (sensitivity analysis) can help direct selection of models and provide feedback to site characterization and facility design steps of the first task. This thorough approach also helps verify the correctness of the analysis.

Task 5 requires that the results from all significant scenarios be combined and compared with the regulations (for example, constructing a complementary cumulative distribution function (CCDF) for assessing compliance with the Containment Requirement of the EPA Standard).

To complete the fourth and fifth tasks, the first three very complex parts must be assembled into an overall, coherent analysis. Several criteria must be met. An analysis must

- Accommodate large uncertainties in input and output
- Permit both uncertainty and sensitivity analyses of models incorporating large discontinuities and nonlinearities
- Be fast running
- Examine a large number of intermediate and final results
- Incorporate quality assurance procedures
- Archive results.

Methods for Performing Tasks

The approach used by Sandia National Laboratories, Albuquerque (SNLA) for meeting these criteria is to

- Use Monte Carlo techniques with efficient Latin hypercube sampling (LHS) to propagate uncertainties
- Modularize the tasks
- Use fast-running mathematical modules or subdomains of the disposal system where appropriate (but not at the expense of important processes)
- Use a neutral file format (such as described below) to provide well-defined interfaces between individual modules of the analysis
- Build quality assurance features into the neutral file and program modules
- Automate the overall analysis as much as possible.

The single most important method used to perform the complex tasks of the compliance assessment (i.e., linking codes, properly identifying Monte Carlo simulations, and controlling data flow) was the fourth item listed, requiring that all intermediate results of computer codes (modules) pass through a neutral file, herein called a computational data base or CAMDAT (Compliance Assessment Methodology Data file). This "zigzag" connection offers five advantages:

- Only one plotting package is needed to display results
- Codes are easily changed to take advantage of a more precise module, a fast running module, or a subdomain of the problem (a truly modular method)

- The order of applying codes is easily changed
- Iterating between results of codes is more feasible (i.e., calibration)
- Design of the controller to automate compliance analysis is facilitated
- Assuring quality is straightforward because all data are in one location.

Neutral File, CAMDAT. The precise structure of the computational data base can vary with applications, but for the complicated task of evaluating compliance of a repository, two main features are required:

- Providing a trail for quality assurance (by listing codes which have written to the data base)
- Providing flexibility, and versatility to handle data from different types of codes (e.g., finite difference and finite element codes).

The first feature requires that any code writing to the file also write a record in the file identifying itself. These records can then be printed out when plotting results. This quality assurance feature is especially important when making numerous Monte Carlo simulations where results may vary only slightly and the analysts can easily misprint and thus misinterpret a simulation.

The second feature requires a versatile file format that has been extensively tested. Typical code linkage in a compliance evaluation requires the following order and types of information

- Geometry data for finite element or finite difference meshes
- Geologic and hydrologic properties of geologic setting and repository/shaft
- Model boundary conditions
- QA information
- Results (e.g., fluid fields and pressures) from fluid flow models
- Initial concentrations from source-term models
- Description of a particle pathway and nuclide concentrations from transport models.

A complicating factor is that up to three different model scales are used: regional, local, and repository. Each model stores similar results. Furthermore, results from the regional, local, and repository models must be accessible to the other codes. To handle this problem, the computational data base is composed of three separate files, all with the same format but with a file header indicating the model scale.

CAM Controller, CAMCON. The Compliance Assessment Methodology Controller (CAMCON) is required to allow an analyst to properly build and execute portions or all of a compliance assessment for any specific scenario. Assessing any one scenario may or may not be rapid with CAMCON, however,

because the difficulty and time required are dependent on the data requirements and complexity of the models (either analytic or numerical) chosen as components in the compliance evaluation. In a sense, the level of complexity of the computer models chosen determines how friendly CAMCON is to use.

However, the varying complexity of CAMCON is not a shortcoming. Indeed, the truly modular aspects of CAMCON and the Waste Isolation Pilot Plant Compliance Assessment Methodology permits an analyst to select the proper mathematical rigor when analyzing the conceptual model of the site.

In summary, assembling the tools for the compliance assessment tasks is multidisciplinary, requiring numerous codes and analysts. Assuring the quality of the assessment requires that the flow of data and linkage of codes be well defined and precisely controlled during execution. Furthermore, the need to analyze many different scenarios using different computer codes requires a flexible data linkage.

Nomenclature

Mathematical Symbols

b_i	-	standardized regression coefficient
c_i	-	$\partial R(X_o)/\partial x_i$, function slope at X_o
F_ℓ	-	function representing ℓth consequence module of CAM
I_i	-	measure of importance
L_i	-	release limit for radionuclide i (from Table 1, Appendix A, *40 CFR 191)*
n_r	-	number of radionuclides released from repository
n_s	-	number of mutually-exclusive release scenarios
n_v	-	number of sampling vectors from Monte Carlo (LHS) sampling
n_α	-	number of varying parameters
$P(\hat{R}_k>R)$	-	probability of $\hat{R}_k > R$
$P(\hat{R}_k>R \mid S_j)$	-	conditional probability of $\hat{R}_k > R$ given scenario S_j occurs
$P(S_j)$	-	probability of scenario S_j occurring over 10,000 yr
Q_{i_k}	-	predicted cumulative release for radionuclide i for run k
q_{i_k}	-	predicted release at time t for radionuclide i for run k
R	-	release limits for EPA sum *(40 CFR 191)*
$\hat{R}_k$	-	calculated summed normalized releases (EPA sum) for sample run k
S_j	-	scenario j
S(q)	-	standard deviation of calculated EPA sum predicted release, q
$S(x_n)$	-	standard deviation of variable x_n
$t_{1/2}$	-	radionuclide halflife
x_n	-	variable

Acronyms and Initialisms

ASCII	-	American Standard Code for Information Interchange
ALGEBRA	-	support module for manipulating data in CAMDAT
CAM	-	compliance assessment methodology
CAMCON	-	Compliance Assessment Methodology Controller--controller (driver) for compliance evaluations developed for WIPP
CAMDAT	-	Compliance Assessment Methodology Data--computational data base developed for WIPP (modification of GENESIS and EXODUS)
CCDF	-	complementary cumulative distribution function

40 CFR 191	-	Code of Federal Regulations, Volume 40, Part 191
CH	-	contact handled
DOE	-	(U.S.) Department of Energy
DRZ	-	Disturbed Rock Zone
EEG	-	Environmental Evaluation Group
EPA	-	(U.S.) Environmental Protection Agency
EXODUS	-	computational data base file format for post processors developed by SNLA
FD	-	Finite Difference numerical analysis
FE	-	Finite Element numerical analysis
50 FR 38066	-	Federal Register, Volume 50, page, 38066
Fm.	-	Formation
GENESIS	-	computational data base file format for preprocessors developed by SNLA
HLW	-	high-level waste
IGIS	-	interactive graphics information system
LHS	-	Latin hypercube sampling (efficient, stratified Monte Carlo sampling)
NAS	-	National Academy of Sciences
NEA	-	Nuclear Energy Agency (Paris)
NEFTRAN	-	NEtwork Flow and TRANsport program
NEPA	-	National Environmental Policy Act in 1970 (Public Law 91-190)
NRC	-	(U.S.) Nuclear Regulatory Commission
NWPA	-	Nuclear Waste Policy Act (Public Law 97-425 & 100-203)
PA	-	performance assessment
PRA	-	probabilistic risk assessment
QA	-	quality assurance
RCRA	-	Resource, Conservation, and Recovery Act of 1976 (Public Law 94-580)
RH	-	remote handled
SCP	-	site characterization plan
SEIS	-	Supplemental Environmental Impact Statement
SRC	-	standardized regression coefficients
SNLA	-	Sandia National Laboratories, Albuquerque, NM
SWIFT II	-	Sandia Waste-Isolation, Flow and Transport model solving transient, three-dimensional coupled equations for fluid flow, heat transport, brine miscible displacement, and radionuclide miscible displacement
TRU	-	transuranic

WIPP - Waste Isolation Pilot Plant

YMP - Yucca Mountain Project (formally Nevada Nuclear Waste Storage Investigations)

Definitions

Accessible Environment - "The accessible environment means (1) the atmosphere, (2) land surfaces, (3) surface waters, (4) oceans, and (5) all of the lithosphere that is beyond the controlled area" *(40 CFR 191.12[k])*.

Barrier - "Barrier means any material or structure that prevents or substantially delays movement of water or radionuclides toward the accessible environment. For example, a barrier may be a geologic structure, a canister, a waste form with physical and chemical characteristics that significantly decrease the mobility of radionuclides, or a material placed over and around waste, provided that the material or structure substantially delays movement of water or radionuclides" *(40 CFR 191.12[d])*.

Benchmarking - The comparison of predictions made with one computer code with other codes, which possibly use other numerical or mathematical formulations. Verification (and occasionally validation) exercises use benchmarking studies.

Calibration - The process of fitting parameters in computer models to reproduce observed data.

Compliance Evaluation or Assessment - The process of assessing the overall compliance of a system with specific performance measures. For this report, the system is a deep, geologic disposal repository of the EPA High-Level Waste Standard; the performance measures, the EPA High-Level Waste Standard.

Computer Model - The appropriately coded analytical, quasi-analytical, or numerical solution technique used to solve the mathematical model.

Conceptual Model - The set of hypotheses and data that postulates the description and behavior of the disposal system (e.g., structural geometry, material properties, and all significant physical processes that affect behavior). For WIPP, the data pertinent for a conceptual model are stored in the secondary data base. Several secondary data bases exist since each scenario may have a slightly different conceptual model.

Controlled Area - "The controlled area means (1) a surface location, to be identified by passive institutional controls, that encompasses no more than 100 km^2 and extends horizontally no more than 5 km in any direction from the outer boundary of the original location of the radioactive wastes in a disposal system; and (2) the subsurface underlying such a surface location" *(40 CFR 191.12[g])*.

Disposal - "Disposal means permanent isolation of spent nuclear fuel or radioactive waste from the accessible environment with no intent of recovery, whether or not such isolation permits the recovery of such fuel or waste. For example, disposal of waste in a mined geologic repository occurs when all of the shafts to the repository are backfilled and sealed" *(40 CFR 191.02[l])*.

Disposal System - "Any combination of engineered and natural barriers that isolate[s] spent nuclear fuel or radioactive waste after disposal" *(40 CFR 191.12[a])*. The natural barriers extend to the accessible environment.

Management - "Management means any activity, operation, or process (except for transportation) conducted to prepare spent nuclear fuel or radioactive waste for storage or disposal, or the activities associated with placing such fuel or waste in a disposal system" *(40 CFR 191.02[m])*.

Mathematical Model - The mathematical representation of a conceptual model (Silling, 1983) (i.e., the coupled algebraic, differential, or integral equations with proper boundary conditions that approximate the physical processes in a specified domain of the conceptual model).

Passive Institutional Control - "Passive institutional control means (1) permanent markers placed at a disposal site, (2) public records and archives, (3) government ownership and regulations regarding land or resource use, and (4) other methods of preserving knowledge about the location, design, and contents of a disposal system" *(40 CFR 191.12[e])*.

Performance Assessment - "The process of assessing the compliance of a deep, geologic, waste repository with the containment requirements of *40 CFR 191 Subpart B*. Specifically, performance assessment means an analysis that (1) identifies the processes and events that might affect the disposal system, (2) examines the effects of these processes and events on the performance of the disposal system, and (3) estimates the cumulative releases of radionuclides, considering the associated uncertainties caused by all significant processes and events. These estimates shall be incorporated into an overall probability distribution of cumulative release to the extent practicable" *(40 CFR 191.12[q])*.

Risk Assessment - Risk assessments estimate effects of a substance or process on individuals or an entire population.

Risk Assessment Policy - Risk assessment policy establishes philosophy used to select among analysis choices.

Risk Management - Risk management is the process of evaluating and selecting alternative courses of action.

Scenario - A scenario is a sequence of events and processes, either singly or in combination, that could contribute to the release of radionuclides into the accessible environment.

Significant Source of Groundwater - "Significant source of ground water means: (1) An aquifer that: (i) Is saturated with water having less than 10,000 milligrams per liter of total dissolved solids; (ii) is within 2,500 feet of the land surface; (iii) has a transmissivity greater than 200 gallons per day per foot, Provided, that any formation or part of a formation included within the source of ground water has a hydraulic conductivity greater than two gallons per day per square foot; and (iv) is capable of continuously yielding at least 10,000 gallons per day to a pumped or flowing well for a period of at least a year; or (2) an aquifer that provides the primary source of water for a community water system as of the effective date of this subpart" *(40 CFR 191.12[n])*.

Special Source of Groundwater - "Special source of ground water means those Class I ground waters identified in accordance with the Agency's Ground-Water Protection Strategy published in August 1984 that: (1) are within the controlled area encompassing a disposal system or are less than five kilometers beyond the controlled area; (2) are supplying drinking water for thousands of persons as of the date that DOE chooses a location within that area for detailed characterization as a potential site for a disposal system (e.g., in accordance with Section 112(b)(1)(B) of the *NWPA* and (3) are irreplaceable in that no reasonable alternative source of drinking water is available to that population" *(40 CFR 191.12[o])*.

Transuranic Radioactive Waste - "Transuranic radioactive waste means waste containing more than 100 nanocuries of alpha-emitting transuranic isotopes, with half-lives greater than twenty years, per gram of waste, except for: (1) High-level radioactive wastes; (2) wastes that the Department has determined, with the concurrence of the Administrator, do not need the degree of isolation required by this part; or (3) wastes that the Commission has approved for disposal on a case-by-case basis in accordance with *10 CFR Part 61*" *(40 CFR 191.02[i])*.

Undisturbed Performance - "Undisturbed performance means the predicted behavior of a disposal system, including consideration of the uncertainties in predicted behavior, if the disposal system is not disrupted by human intrusion or the occurrence of unlikely natural events" *(40 CFR 191.12[p])*.

Validation - The process of assuring through sufficient testing (subjective) with real site data that a conceptual model and the corresponding mathematical and computer models correctly simulate a physical process sufficiently accurately (subjective) (Hoffman and Gardner, 1983; Silling, 1983).

Verification - The process of assuring (e.g., through tests on ideal problems) that the computer code correctly solves the mathematical model. Given that a code correctly solves the mathematical model, the physical assumptions must be checked through validation.

Review and Discussion of Code Linkage and Data Flow in Nuclear Waste Compliance Assessments

1. Introduction

1.1 Purpose and Organization of Report

The purpose of this report is to describe the complex flow of data that occurs when evaluating the compliance of a deep, geologic nuclear waste repository with U.S. government regulations.

To meet this purpose, this report has two main sections. The first section, background information on assessing compliance of repositories, is discussed in Chapters 2 and 3, which

- Review basic concepts used in detailed assessments and the Environmental Protection Agency (EPA) Standards for high-level waste (HLW) repositories (Chapter 2)
- Review of Sandia National Laboratories-Albuquerque's (SNLA's) systematic approach to evaluating compliance with EPA Standards (Chapter 3).

The second section, composed of Chapters 4, 5, and 6, describes the sequence in which data are generated and the necessary flow of data implied by the CAM. In essence, the chapters of this section provide a concrete description of the procedure used and the magnitude of the problem:

- Description of components of CAM that impact the flow of data (Chapter 4)
- General description of method used to pass data between components of CAM (Chapter 5)
- Detailed description of the flow of data using SNLA's CAM (Chapter 6).

Appendices A and B discuss the computational data base and the secondary data base, respectively.

Each chapter generally builds upon concepts introduced in the preceding chapter. If you are familiar with the concepts of compliance assessments, after reading this introduction (and possibly skimming over the figures in Chapters 2 and 3) skip to Chapters 4, 5, and 6. If you are unfamiliar with compliance assessments and want to understand the motivation behind the data flow described in Chapters 5 and 7, read Chapters 2 (very basic) and 3.

1.2 Objective of Code Linkage

Purpose. Besides providing a detailed review, this report describes the flow of data and linkage of consequence analysis computer codes for assessing compliance of deep, geologic waste repositories primarily, the Containment Requirements in Subpart B of the Code of Federal Regulations, Title 40, Part

191 (*40 CFR 191*), which were promulgated by the EPA. By describing the flow of data, the specific algorithm used is thereby defined.

Need for Data Control. Assessing the regulatory compliance of a geologic repository is a multidisciplinary project, requiring the use of numerous codes and personnel to predict probabilities and amounts of radioactive release outside the controlled area of a repository. Consequently, assuring the quality of the assessment requires that the flow of data and linkage of codes be well defined for the assessment procedure and precisely controlled during execution.

For example, transferring data from one code to another is subject to human error. In addition, evaluating the uncertainty of the results because of uncertainty in model parameters requires numerous repetitions, compounding the chance for errors. Furthermore, results from these repetitions must be plotted and properly identified to distinguish simulations.

Scope of the Report. In this report, emphasis is placed on the manner of linking codes and the data bases necessary for improving the quality of evaluations when assessing repository performance, rather than on any specific computer codes used. Consequently, this is not a user's guide (however, see Rechard, 1989). Furthermore, although the code linkage and data flow described herein were specifically developed for deep geologic waste disposal performance assessments, the concepts are quite general, with applicability not only to other types of risk assessments but whenever code coupling is required (for example, coupling predictions from large-scale atmospheric or oceanic forecast models with detailed regional forecast models).

Although the individual code linkage and data flow components are general and could be described with generic examples, many of the difficulties, and thus the need for subtle features, are evident only during an actual assessment of a geologic repository. Therefore, the examples all pertain to the Waste Isolation Pilot Plant (WIPP) project, which prompted development of the concepts. A section in this introduction provides background information on the WIPP site.

1.3 Relationship with Previous Performance Assessment Work

SNLA has been developing tools and procedures for assessing the safety of HLW in hypothetical repositories in bedded salt and basalt for a number of years for the Nuclear Regulatory Commission (NRC) (Campbell and Cranwell, 1988; Cranwell et al., 1987; Bonano et al., 1988). These studies simulated a steady-state groundwater flow field, evaluated a particle pathway, and then calculated radionuclide transport along this pathway from a simple source.

SNLA has also been involved with assessing the feasibility of disposal of HLW in the subseabeds of the deep oceans for the Department of Energy (DOE) and the international Nuclear Energy Agency (NEA) of the Organization for Economic and Cooperative Development, Paris (e.g., de Marsily et al.; NEA, 1988. The approach used in the performance assessment was to start with a repository model containing detailed physical/chemical processes (Hickerson et al., 1988; Lanza, 1988) and continue with both

transient fluid flow and transport through successive barriers (Shephard et al., 1988; Marietta and Simmons, 1988; Pentreath et al., 1988; Brush, 1988), culminating in a dose assessment.

Although the flow of data and specific algorithms described in this report are consistent with previous work, the tools previously developed were often exploratory, being for hypothetical repositories. The compliance evaluation tools described here are applicable to a real site; thus, many modeling problems are solved for the first time. For example, because compliance assessments involve a significant amount of work, assuring the quality and the flexibility of the analysis is a very important component of the methodology described in this report.

Consequently, the work reported here builds upon previous concepts, while discarding many specific tools of previous work. The experience and new tools developed for the WIPP can easily contribute to both the efforts of the NRC to regulate a DOE commercial repository and to the NEA's feasibility studies for subseabed disposal.

1.4 Evaluating Compliance with the EPA Standard

EPA Standard (40 CFR 191). The EPA Standard, *Environmental Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level, and Transuranic Radioactive Wastes (40 CFR 191),* is divided into two subparts. Subpart A limits annual radiation doses to the public during active operation of the disposal facility. Subpart B limits total releases of radionuclides into the accessible environment for 10,000 yr, radiation doses to the public for the first 1,000 yr, and radioactive contamination of special sources of groundwater for the first 1,000 yr. Assessment of compliance with Subpart A is primarily through air quality monitoring. Assessment of compliance with Subpart B is primarily through an extensive performance evaluation. Guidance for performing the Subpart B assessment is contained in Appendix B of the EPA Standard, the cumulative release limits over 10,000 yr being the requirement most influencing the methods used.

SNLA Compliance Evaluation. Based on previous work (e.g., NEA, 1988; Helton et al., 1988; Cranwell et al., 1987), SNLA has developed a systematic method for assessing compliance with the release limits in Subpart B. The method has five major tasks:

- Collecting data on waste properties, site geology and hydrology, and preliminary facility design to characterize the disposal system and surrounding area
- Identifying the events and processes whereby radionuclides may be released into the accessible environment
- Predicting the amount of these releases through modeling
- Evaluating the uncertainties associated with these predictions and the most important variables which influence these uncertainties
- Comparing the predicted releases with government regulations.

The complete assembly of the tools to perform the latter three tasks in the assessment is described in this report. Generally, Task 3 requires the use of many different codes, each using different solution

methods and computational subdomains of the disposal system that must be linked together. For example, groundwater flow can be simulated at two scales, regional and local. Also, the repository/shaft system model must be coupled with the local-scale groundwater flow model.

Task 4 of SNLA's methodology requires that uncertainties be propagated through the analysis and that the important parameters influencing these uncertainties be identified. The approach described in this report relies heavily upon Monte Carlo techniques using efficient Latin hypercube sampling (LHS) (Iman and Conover, 1980).

Task 5 requires that the results from all Monte Carlo simulations of each of the significant scenarios be combined to allow comparison with the regulations. SNLA's approach for the Containment Requirements is to produce a complementary cumulative distribution function (CCDF) as suggested in Appendix B of the EPA Standard. The Individual Protection Requirements are treated as a special case of the Containment Requirements. The Groundwater Protection Requirements could also be treated as a special case. This treatment is unnecessary for WIPP, since no special groundwater is present (WIPP Strategy, 1988).

1.5 Methods Used to Perform Compliance Assessment

General Approach. SNLA's general approach to the latter three tasks of compliance assessment is to

- Use Monte Carlo techniques for propagating uncertainties in Task 4
- Modularize the tasks in the consequence analysis
- Use fast-running mathematical models or computationally efficient subdomains of the disposal system where appropriate in Task 3
- Build in quality assurance (QA) features for data control
- Automate the overall analysis as much as possible
- Use a neutral file format (described later) to provide well defined interfaces between individual modules.

Linking Codes and Controlling Data Flow. The single most important technique used in performing the complex tasks of the compliance assessment (e.g., linking codes, properly identifying Monte Carlo simulations, and controlling data flow) is the last item listed, requiring that all intermediate results of modules (individual computer code) pass through a neutral file, herein called a computational data base (Figure 1.1). This feature makes it possible to easily incorporate other necessary tasks and features.

To illustrate, having one neutral file (the computational data base) through which all data pass facilitates design of the executive driver, Compliance Assessment Methodology Controller (CAMCON) (Rechard, 1989), needed to automate much of the analysis. Furthermore, information on each Monte Carlo simulation for a scenario is stored in one location, guaranteeing reproducibility of the simulation if necessary--an important requirement of QA.

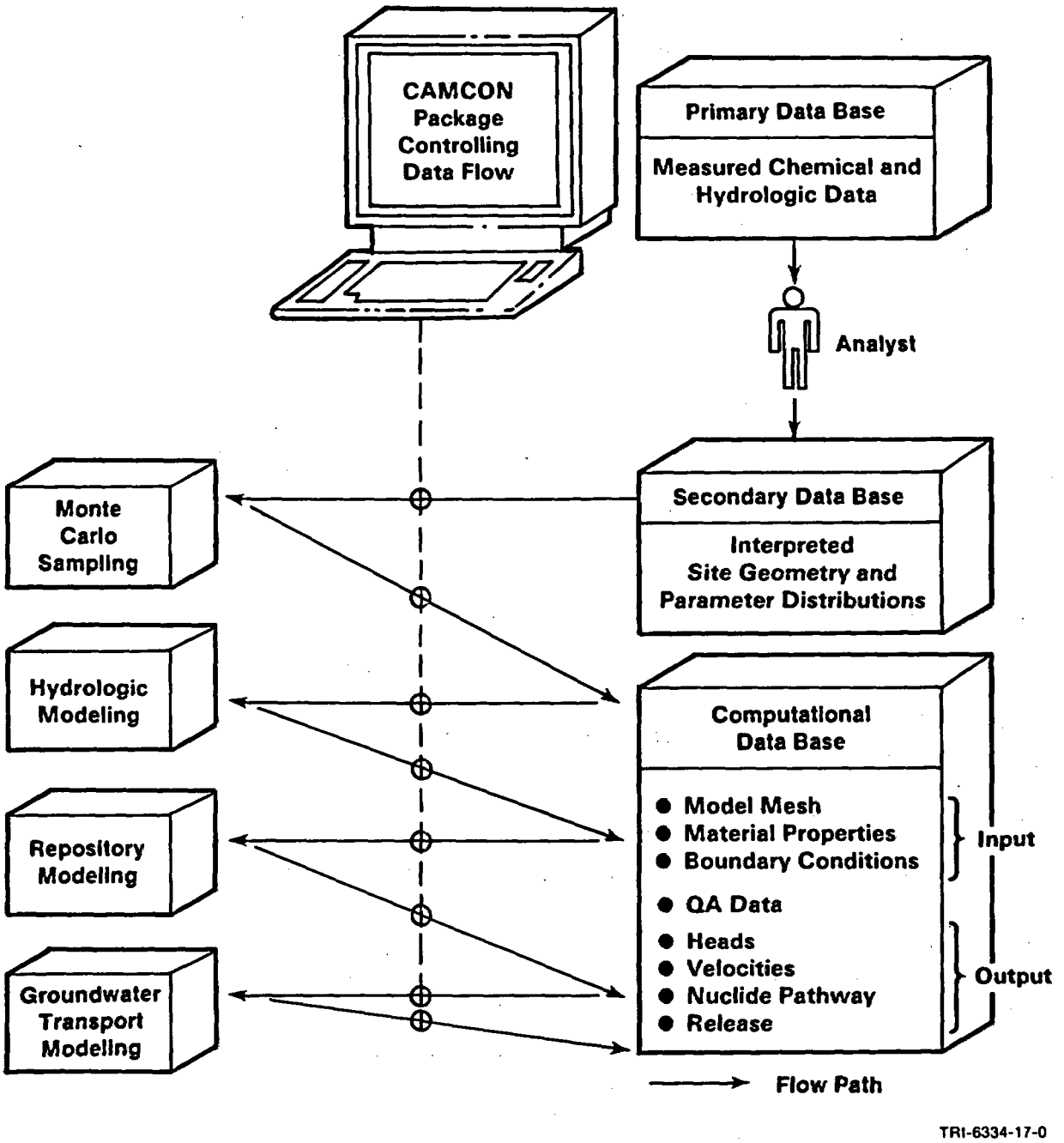

Figure 1.1 Code linkage and data flow in nuclear waste compliance assessments.

With this approach, steps in the consequence analysis are truly modular (not just conceptually, but practically as well), because all system modules communicate through the computational data base rather than directly with each other.

For example, for any one scenario, the consequence analysis typically requires different model complexities for the underground facility, groundwater flow, or transport of radionuclides (Figure 1.1). A new module can be substituted easily to take advantage of a more precise module, a fast running module, or a more computationally efficient subdomain of the problem (new translators to and from the module may be necessary, but the specifications to the programmer are clear, speeding up development).

For completeness, data flow from the two other major data bases needed in compliance assessment is also depicted in Figure 1.1. The primary data base consists of site-specific data strictly controlled to assure quality. The analysts use this data (along with professional judgment, etc.) to develop a conceptual model of the disposal system, embodied in the secondary data base. This secondary data base is then accessed by the executive controller, CAMCON, during one simulation of a scenario.

1.6 Background on WIPP

As previously mentioned, the WIPP provided the impetus for assembling various performance assessment concepts (e.g., NEA, 1988; Cranwell et al., 1987) that have been developed. The WIPP also serves as the primary illustration in this report. Brief information on the WIPP follows.

Purpose. The WIPP is a full-scale pilot plant originally planned to demonstrate

- The safe management, storage, and disposal of the transuranic (TRU) waste (disposal only after compliance with the EPA Standard has been demonstrated)
- The safe management and storage (but not permanent disposal) of HLW from defense activities of the U.S. DOE exempted from regulation by the NRC (Pub. L. 96-164, 1979).

The second task is no longer needed because of the decision of Congress to place U.S. commercial waste in volcanic tuff at Nevada; hence, this task is being phased out (Pub. L. 100-203, 1987).

In late 1989, the WIPP is scheduled to begin emplacing a limited amount of transuranic (TRU) waste generated by nuclear weapon facilities for a 5-yr pilot phase. This waste consists of laboratory and production trash such as glassware, metal pipes, disposable laboratory clothing and gloves, cleaning rags, solidified sludges, and so on contaminated with TRU radionuclides (e.g., plutonium). Between 60 and 85% may also be contaminated with hazardous waste (RCRA, 1976). By regulatory definition, TRU waste has a curie content greater than 100 nCi/g. Waste contaminated with less than 100 nCi/g is low-level or mixed waste and is disposed at near-surface landfills.

Although only about one-third of the waste currently exists, if licensed, the WIPP will ultimately dispose of about 1.2×10^5 m^3 (4.4×10^6 ft^3) of TRU waste that can be contact handled (CH). For CH-TRU waste, the external dose is low so that personnel can handle sealed containers without special precautions. The CH-TRU waste consists of about 3.8×10^5 0.21-m^3 (55 gal) steel drums, 6×10^3 3.2-m^3 steel and plywood boxes, and 1.35×10^4 1.8-m^3 steel boxes (IDB, 1988). As an example, for this CH-TRU waste 4.7×10^6 kg (1.0×10^7 lb) is cellulose (e.g., paper, cloth, and lumber) with 20% from the containers and 2.4×10^7 kg (5.3×10^7 lb) is steel with 67% from the containers (33% in contents). The total curie

content of the CH-TRU waste is about 9.4 x 10^6 Ci. Although a room can ideally store about 6800 drums stacked three deep, each of the underground rooms and drifts (56 rooms and about 56 room equivalents, respectively) will contain a repository average of about 5300 drum equivalents.

A small portion of the TRU waste must be remote handled (RH); that is, transported and handled in shielded casks. The contents are being determined, but must be less than 5.1 x 10^6 Ci according to the agreement between the DOE and the State of New Mexico (DOE/NM, 1984). The shielded casks will be emplaced in horizontally drilled holes in the walls of the rooms. All CH and RH TRU waste packages must meet the WIPP Waste Acceptance Criteria (WEC, 1985) and must be certified for shipment to the WIPP.

Location. The WIPP site is about 26 mi east of Carlsbad, NM (Figure 1.2). The site was chosen because of the 2000-ft-thick Salado and 1000-ft-thick Castile bedded salt formations. The bedded salts consist of thick halite and minor clay and anhydrite strata, approximately 200 million yr old, that do not contain flowing water. The repository level is near the center of these strata, 2150 ft below the surface and 1300 ft above sea level (Figure 1.3). Water-bearing units (primarily the Culebra Dolomite) in the Rustler Formation (Fm.) above the Salado Fm. produce only small amounts of water, too salty for human consumption. Pockets of brine under pressure may occur well below the repository horizon within the Castile formation. The Pecos River, 14 mi away, is the nearest perennial stream (Bertram-Howery and Hunter, 1989).

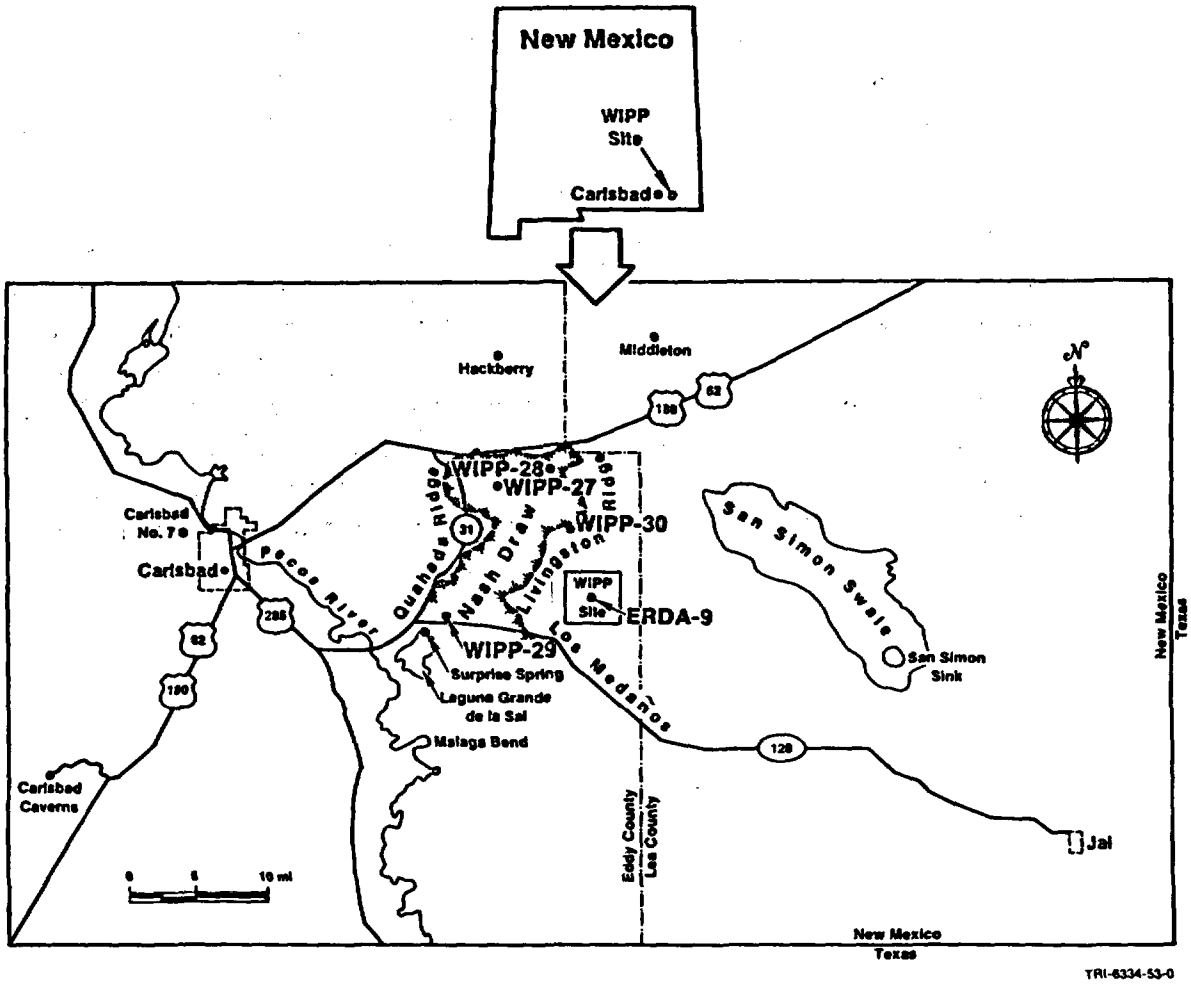

Figure 1.2 Location of the WIPP site in southeastern New Mexico (after Lappin, 1988).

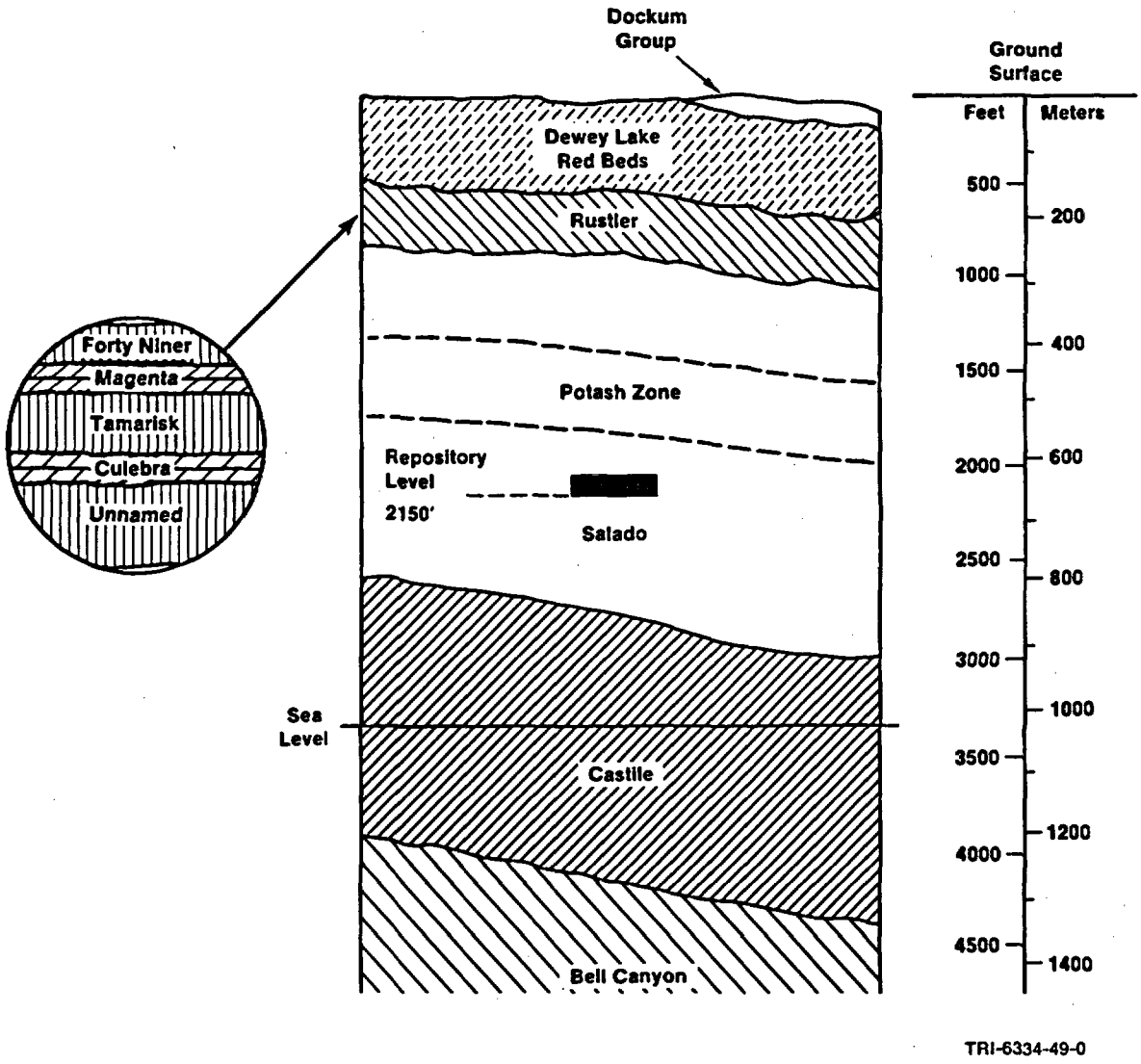

Figure 1.3 General stratigraphy at the WIPP site (after Lappin, 1988).

SNLA Role in Project. Three major participants support DOE in the WIPP project (WIPP Strategy, 1988) (Figure 1.4):

- SNLA functions as scientific investigator and advisor
- Westinghouse Electric Corporation is responsible for WIPP site operations
- Bechtel, Inc. is responsible for design and inspection.

DOE Headquarters has responsibility for determining regulatory compliance of WIPP. External to the DOE, the WIPP project is reviewed by the State of New Mexico's Environmental Evaluation Group (EEG) and the National Academy of Sciences (NAS) WIPP Panel.

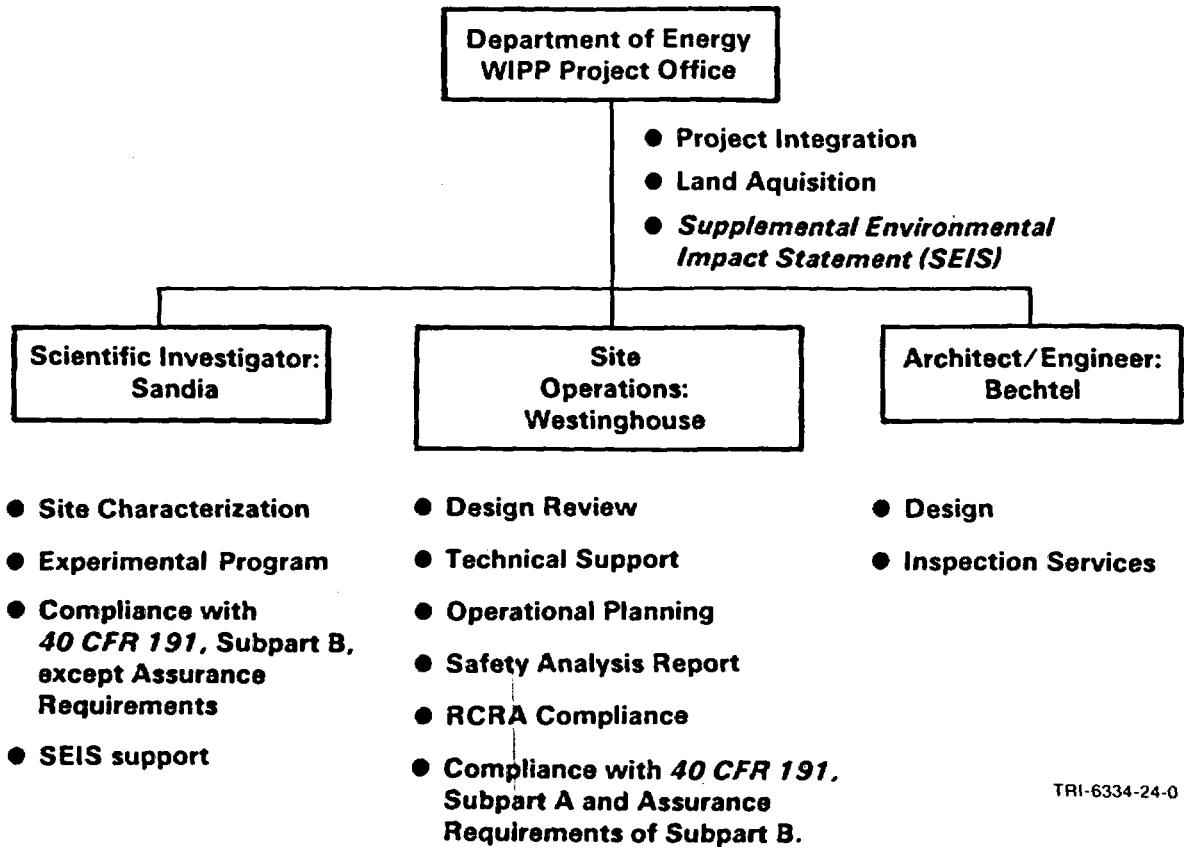

Figure 1.4 Responsibilities of participants in the WIPP project (after WIPP Strategy, 1988).

The specific tasks of SNLA are (Figure 1.4)

- Characterizing the site and responding to specific concerns of the State of New Mexico
- Performing field experiments to support site characterization and applied research
- Providing support for the *Supplemental Environmental Impact Statement (SEIS)*
- Ensuring regulatory compliance with Subpart B of *40 CFR 191* except for the Assurance Requirement.

This report helps fulfill the last task (not assigned to SNLA until October 1986).

Influence of EPA Standard. Preliminary work on at the WIPP site began in 1975, before the concepts of compliance assessment were fully developed. Based on early criteria developed by the NAS, the WIPP site was selected and an Environmental Impact Statement completed in 1980 which showed hypothetical releases would be below background levels (DOE/EIS, 1980). Although DOE has always striven to construct a safe repository, the EPA Standard promulgated in September 1985 more thoroughly defined the criteria for what constitutes a safe site and required a careful evaluation of predicted performance. Consequently, the task has greatly influenced the other two functions assigned to SNLA, site characterization and field experiments.

2. Assessing Compliance of Deep Geologic Repositories

This chapter provides a basic review of

- Risk assessment concepts
- Legislative performance measures that must be addressed
- Sources of uncertainty.

This review is necessary for understanding the data flow and code linkage required in a compliance assessment.

If you have had an introduction to these subjects, you may wish to skip to Chapter 3, which discusses methods for evaluating the performance of a repository against these criteria. Otherwise, use Chapter 2 as a cursory review of pertinent regulations and technical problems that must be addressed.

2.1 Risk Assessment in General

Background on Risk Assessment. The need for assessing risks to the public has coincided with the growing public expectation that a government should protect its citizens against not only acute (immediate) hazards, but chronic (long-term) hazards as well (Risk Assessment, 1983). The concern that ionizing radiation causes cancer contributed to this expectation.

The current methods for assessing these risks have evolved from several events and the responses to these events (Kaye, 1983). An important first event was nuclear weapons production. The accompanying response was monitoring of radionuclide releases from production facilities in the late 1940s and the measurements of worldwide fallout from atmospheric testing in the early 1950s. Another event, the proposed peaceful use of nuclear explosives (Plowshare Program) in the late 1950s, created a need for predicting movement and attendant health risks of radionuclides that might vent to the atmosphere or enter the groundwater. Application during the 1960s of engineering systems analysis (developed for evaluating large systems such as reactors) was the response to this problem.

The National Environmental Policy Act (NEPA) of 1969 mandating government agencies to evaluate the long-term impact of technological initiatives on the biologic, social, and economic environment was an event that caused several responses. The NEPA acknowledged that technology created side effects and that all alternatives should be examined to more adroitly direct technology (Wenk, 1986). More stringent requirements for pollutants indirectly resulted from the NEPA. These more stringent requirements, in turn, require more realistic analysis, not just highly conservative analysis.

As interpreted by the Atomic Energy Commission, the phrase "long-term impact" included long-term health effects. Hence the *Reactor Safety Study* (NRC, 1975), a comprehensive effort to examine long-term impacts using system analysis, introduced and developed the concept of a probabilistic risk assessment (PRA). Although widely heralded as a significant contribution, reviewers criticized its failure to

characterize uncertainties in the results (Helton et al., 1988). Realistic analysis, unlike conservative analysis, requires evaluating the uncertainty associated with predictions.

These PRA concepts, along with uncertainty analysis, were extended to geologic repositories and subseabed disposal (Cranwell et al., 1987; NEA, 1988). Regulations for TRU and high-level radioactive waste disposal promulgated by the EPA (40 CFR 191) currently require a risk-based, systems-analysis approach for assessing compliance of nuclear waste repositories with long-term release limits.

In general, the PRA methodology has been applied to diverse problems to aid in decision-making where health risks are concerned. Such results are often needed early in a project when very little detailed information is available, but the glimpse gained from the analysis is still useful (Rechard et al., 1988).

Definitions. The procedure outlined in Chapter 3 is not a PRA, but does make use of PRA concepts. PRA techniques have matured rapidly in the past decade; however, definitions do vary. Hence, definitions below are used in this report.

Risk.. Risk is defined as the product of the probability of an event or process times the effect or consequence of that event or process.

Risk Assessments. Risk assessments estimate probabilities and effects or consequences of a substance or process on an individual or population (Risk Assessment, 1983).

Risk Management. Risk management is the process of evaluating and selecting alternative courses of actions. A primary component of the decision criteria is the factual input provided by a risk assessment but regulations, public issues, feasibility, and costs are also important considerations. Ideally, risk assessments should be completely separated from risk management decisions (Risk Assessment, 1983).

Risk Assessment Policy. Professional judgment, experience, and consensus must bridge the gaps in knowledge that invariably exist in risk assessments. Risk assessment policy establishes the philosophy used to select methods and analysis choices. For example, policy establishes the degree of conservatism in a risk assessment if there is no decisive way to make the choice between several analysis options. Although seemingly containing aspects of risk management, risk assessment policy is always subordinate to scientific fact (Risk Assessment, 1983).

Policy also establishes the use of expert opinion. For example, determining the amount of data that is sufficient and the interpretation of those data to produce conceptual models for each release scenario at a site requires expert opinion. Furthermore, assigning probabilities to rare events or judging the adequacy of model validation also requires expert opinion.

For nuclear waste disposal, the risk assessment policies are highly formalized, requiring extensive documentation describing

- Criteria for selecting experts (e.g., required knowledge; ensuring that all disciplines are adequately represented on multidisciplinary questions)
- Why scientific facts alone cannot be used to bridge data gaps
- How consensus was reached among the experts
- Documentation of dissenting views
- How new data might alter expert opinions.

2.2 Regulatory Requirements For Geologic Repositories

The intent of the *40 CFR 191* Standard is

- To provide an achievable level of protection, given the existing disposal alternatives
- To reduce the risk from nuclear waste to future generations to "acceptably" low levels.

The latter purpose is accomplished by isolating the wastes for a significantly long time, specifically by reducing the risk so that it is not greater than if the source of the waste, uranium ore, had not been mined *Federal Register, Volume 50,* page 38066 *[50 CFR 38066]).* The following text provides an overview of the pertinent EPA and NRC regulations. For specifics, refer to the regulations themselves *(40 CFR 191 and 10 CFR 60).*

EPA Regulations (40 CFR 191). The Standard is divided into two subparts (Figure 2.1). Subpart A limits annual radiation doses to the public outside the secured area ("area under effective control") during the operational life of the facility. Although some projections are necessary for the *Final WIPP Safety Analysis Report* (DOE/FSAR, 1988), annual compliance during the management and storage segment is evaluated primarily from extensive monitoring data in conjunction with the code AIRDOS-EPA (Moore et al., 1979). Consequently, a complex system of computer programs to make predictions is not required and this aspect is not discussed further.

Subpart B establishes post-disposal requirements for containment, assurance (design and control philosophy), individual protection, and groundwater protection (Figure 2.1). The primary goal of Subpart B is to limit long-term releases of certain radionuclides to the accessible environment. Assuring compliance with Subpart B (specifically, the Containment Requirement) is the main reason for the detailed system analysis outlined in this report.

Although in July 1987, the U.S. Court of Appeals for the First Circuit vacated Subpart B and remanded it to the EPA for further consideration, the following discussion concerns Subpart B as first promulgated (the points of major contention were the individual protection dose limits, the 1,000-yr time period, and the Groundwater Protection Requirements).

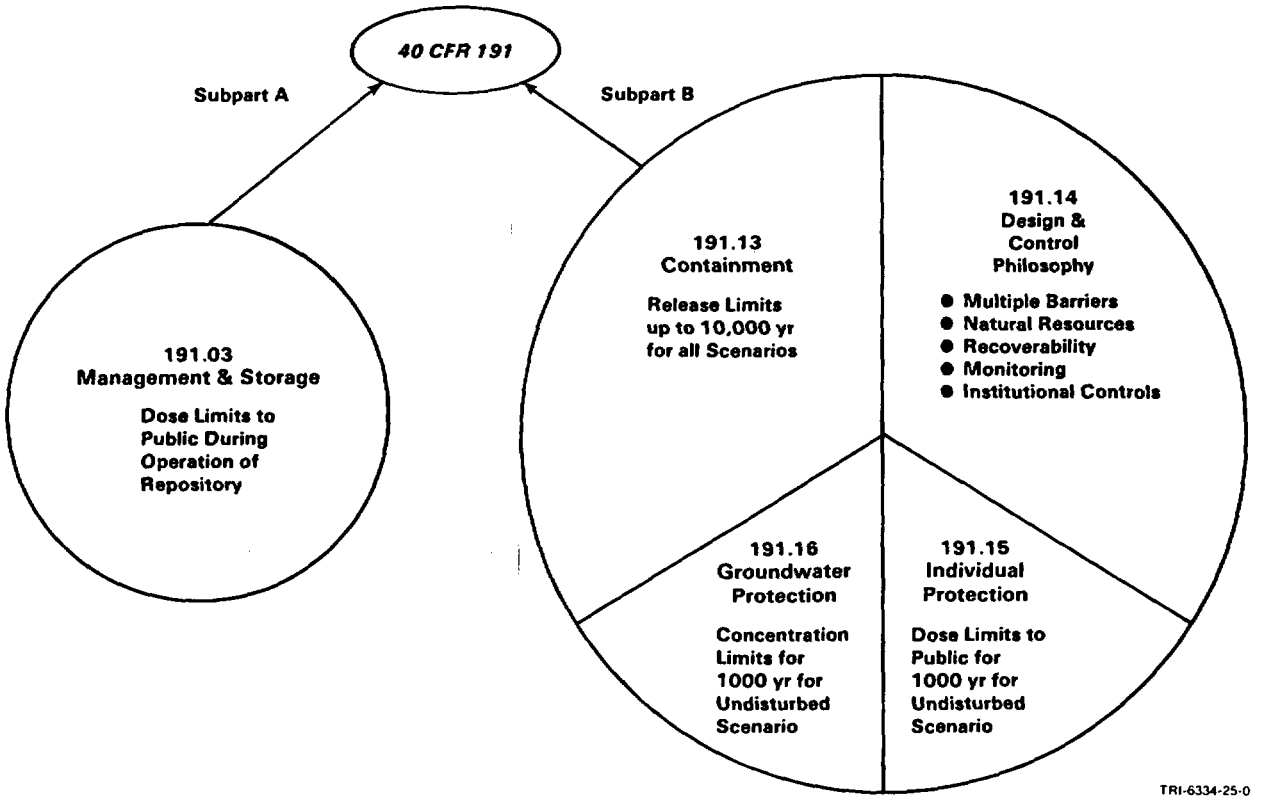

Figure 2.1 Containment and Assurance Requirements are the principal components of the EPA High-Level Waste Standard (after WIPP Strategy, 1988).

Regulatory Definitions. The following text paraphrases definitions found in *40 CFR 191.* Direct quotations of the definitions are in the nomenclature on page xi of this report.

- "Management" includes any activity conducted to prepare TRU waste, HLW, and spent nuclear fuel for storage or disposal and any activity associated with emplacement of waste in a disposal system, exclusive of transportation.
- "Storage" is the retention of nuclear waste with the intent and capability of ready retrieval for subsequent use, processing, or disposal.
- "Disposal" is the permanent isolation from the accessible environment of TRU waste, HLW, and spent nuclear fuel with no intent of recovery after the repository shafts and boreholes are backfilled and sealed.
- "Disposal System" means any combination of engineered and natural barriers that isolates TRU waste, HLW, and spent nuclear fuel after disposal. Because the performance of the system is evaluated at the boundary of the controlled area, in this report the natural (geologic) barrier includes the controlled area.

- "Barrier" means anything that prevents or substantially delays movement of water or radionuclides toward the accessible environment.

- "Accessible Environment" means the atmosphere, land surfaces (including land surfaces within the controlled area), surface water, oceans, and all of the lithosphere beyond the controlled area.

- "Controlled Area" means a surface location and underlying subsurface identified by passive institutional controls that encompass no more than 39 mi^2 (100 km^2) and extends horizontally no more than 3.1 mi (5 km) in any direction from the outer boundary of the original location of the TRU waste, HLW, and spent nuclear fuel. Prior to the complete compliance assessment, only a tentative estimate of the minimum necessary area has been made at the WIPP (WIPP Strategy, 1988).

- "Passive Institutional Control" includes permanent markers placed around the surface perimeter of the disposal system, public records, government ownership, and regulations regarding land and resource use.

- "Undisturbed Performance" means the predicted behavior, including all likely natural processes (not unlikely or human intrusion events) and pathways to man in the accessible environment.

- "Significant Source of Ground water" means an aquifer that is the primary source of water for a community or a potential source of water that (1) contains less than 10^5 mg/ℓ total dissolved solids, (2) is within 2,500 ft (760 m) of the surface, (3) has a transmissivity greater than 200 gal/day/ft (3×10^{-5} m^2/s), (4) has hydraulic conductivity greater than 2 gal/day (3×10^{-5} m/s), and (5) can supply 10^5 gal/day (4×10^{-3} m^3/s) for a year.

- "Special Source of Ground water" means EPA Class I groundwater (EPA, 1984) that is within the controlled area or less than 3.1 mi (5 km) beyond the controlled area, (2) supplies drinking water for thousands of persons at the time the site was selected for characterization, and (3) is irreplaceable to that population.

- "Performance Assessment" means the process of assessing the compliance of a disposal system with the containment section of Subpart B, *40 CFR 191.13* including uncertainties, and developing a probability distribution of cumulative release.

Concerning the last definition, assessing whether a repository meets a set of performance criteria is frequently termed a performance assessment (PA). Unfortunately, the EPA defined this general term to specifically mean assessing compliance with the Containment Requirements of *40 CFR 191,* Subpart B. Consequently, this report avoids using the term PA; rather it uses the term compliance assessment or evaluation when talking about assessing the overall performance of a geologic repository. It uses the term Containment Requirement when referring to the containment section.

Containment Requirements (40 CFR 191.13). The Containment Requirements and the "design philosophy" spelled out in the Assurance Requirements *(40 CFR 191.14)* are the major components of the regulation (Figure 2.1). Specifically, the Containment Requirement requires that a disposal system have a reasonable expectation that the cumulative releases to the accessible environment of one radionuclide from TRU waste, HLW, and spent nuclear fuel for 10,000 yr from all significant processes and events must have (Figure 2.2)

- Less than one chance in 10 of exceeding quantities calculated from Table 2.1 (*40 CFR 191,* Appendix A)

- Less than one chance in 1000 of exceeding ten times those quantities.

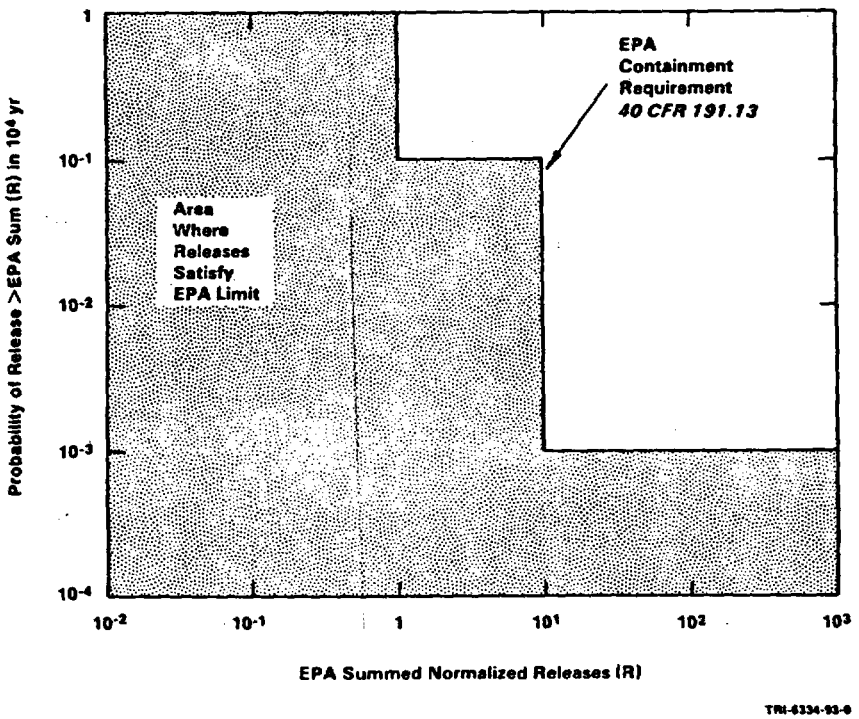

Figure 2.2 Release limits of the Containment Requirements of the EPA Standard are probabilistically based.

Table 2.1 Cumulative release limits, L_i, to the accessible environment 10,000 yr after disposal (*40 CFR 191*, Appendix A).

Radionuclide	Limit, L_i, per 10^6 Ci α-emitting TRU nuclides with $t_{1/2} > 20$ yr* (Ci)
Americium-241 or -243	100
Carbon-14	100
Cesium-135 or -137	1000
Iodine-129	100
Neptunium-237	100
Plutonium-238, -239, -240, or -242	100
Radium-226	100
Strontium-90	1000
Technetium-99	10000
Thorium-230 or -232	10
Tin-126	1000
Uranium-233, -234, -235, -236, or -238	100
Any other α-emitting radionuclide with $t_{1/2} > 20$ yr	100
Any other non-α-emitting radionuclide with $t_{1/2} > 20$ yr	1000

*Other units of waste described in *40 CFR 191*, Appendix A

For a combination of radionuclides, the sum of the releases of all radionuclide normalized with respect to the EPA limits (*40 CFR 191,* Appendix A, Table 3.1) must remain below 1 for events with probabilities of occurrence of one chance in 10 and below 10 for event probabilities of one chance in 1000:

$$\hat{R} = \sum_{i=1}^{n_r} \frac{Q_i}{L_i} \leq 1 \text{ (or 10)} \qquad [1.1]$$

where

L_i = the EPA release limit of radionuclide i (Table 2.1)

n_r = number of radionuclides released or created

Q_i = the predicted release of radionuclide i

$\hat{R}$ = summed normalized releases (EPA sum).

Hence, the Standard has a probabilistic basis (Figure 2.2).

The Standard acknowledges that there will be substantial uncertainties in predicating the disposal-system performance. The Standard requires only a reasonable expectation based on the collected evidence (scientific facts and their interpretation).

Because of the probabilistic and uncertainty requirements implied by the EPA definition of PA in Subpart B, the Containment Requirement *(40 CFR 191.13)* is the most demanding part of the Standard and drives the development of the system. Although the regulations do not specify a probabilistic risk assessment (PRA) method, SNLA's approach for assessing the disposal system resembles a PRA, except that the performance criteria differ. Specifically, SNLA's approach follows the nonbinding guidance provided in Appendix B of *40 CFR 191.*

The procedure was developed simultaneously with early drafts of the regulations and was used to evaluate many options for the NRC and EPA (e.g., Chu et al., 1983; Pepping et al., 1983). However, variations are possible. For example, another procedure might rely more heavily upon stochastic rather than deterministic modeling should stochastic models become readily available.

Rationale for Containment Requirements. Discussion follows of four aspects of the EPA Standard (more detail is found in the preamble published with the final rule [*50 FR 38066*]):

- Performance of the repository as a system
- The 10,000-yr regulatory period
- Assumed predictive capability
- Release limits.

Concerning performance of the repository as a system, the EPA Containment Requirement provides a performance measure for the entire disposal system, not individual components. However, the Assurance Requirements, discussed later, do require a multiple-barrier concept. Furthermore, NRC regulations establish performance requirements for the individual components of the multiple barrier.

The EPA advocated the concept that 10,000 yr is fairly short geologically, so that significant geologic changes would not occur, yet long enough to establish from predictive calculations that the repository location was suitable (*50 FR 38066*). Consequently, the EPA uses a 10,000-yr regulatory period.

Concerning predictive capability, the EPA assumed that predictions about physical phenomena would be adequate for evaluating compliance with the regulations. However, the EPA Standard does not set allowable health risks (i.e., it is not a health standard). Some information necessary for a PRA based on health risks would contain extreme uncertainty (e.g., location of populations in 10,000 yr, the long pathway to this population, or the precise release rate of radionuclides); thus, the regulatory performance measure avoided using these factors. Instead, the EPA developed radionuclide release limits at a specified boundary and human dose limits for the disposal system. Furthermore, to diminish the need for knowing the precise release rate and dispersion of the radionuclides, the cumulative discharge over 10,000 yr, rather than the concentration variation with time, was required.

The release limits for common radionuclides in a waste inventory were established by assessing hypothetical repositories representative of sites under consideration in the early 1980s with engineered barriers as specified in *10 CFR 60* at that time (Smith et al., 1981). Release to the air, land, ocean, and rivers was considered. The river pathway dominated the risk of cancer; this risk was evaluated by assuming that the waste ultimately reached a river and that a population, proportional to the ratio of the flow of all rivers in the world to the entire world population, consumed 2 ℓ/day/person from this river (Helton, 1983).

From this estimated risk, the EPA established limits on radionuclide release to the accessible environment (Table 2.1) that would not cause more than 100 cancer deaths over 10,000 yr per 100,000 metric tons of heavy metal disposed (Helton, 1983). The 100 cancer deaths over 10,000 yr was the estimated risk from unmined uranium ore bodies (Smith et al., 1981). The permitted amount of release is proportional to the amount of waste stored.

Assurance Requirements (40 CFR 191.14). The Assurance Requirements define six criteria for designing and controlling the disposal system. This control philosophy includes

- Maintaining active control over the site as long as possible
- Monitoring the repository area for a reasonable period to check for any deviation from expected performance
- Using passive institutional control to mark and preserve knowledge of the disposal system.

The design philosophy includes

- Using a combination of engineered and natural barriers to isolate wastes from the accessible environment
- Avoiding areas of abundant natural resources to lower the probability of inadvertent human intrusion
- Using a mined geologic repository to permit recovery over a reasonable period of time.

Individual Protection Requirements (40 CFR 191.15). Section 191.15 protects individuals in the population from releases during the first 1000 yr after disposal by limiting the annual dose to any member of the public to 25 mrems to the whole body or 75 mrems to any critical organ, requirements similar to those for nuclear power operators *(40 CFR 190)*. The undisturbed performance (that is, the predicted performance of the disposal system, considering all pathways to man in the accessible environment from release by likely natural processes, but not human intrusion) is used to calculate the dose to an individual. The uncertainties in predicted behavior must be evaluated, but only the median or mean of the resulting distribution of radiation exposures is compared with the stated limits, not the whole distribution, as for the Containment Requirements.

Groundwater Protection Requirements (40 CFR 191.16). Section 191.16 specifically protects special sources of groundwater within or near the controlled area. During the first 1000 yr after disposal, concentrations of radionuclides in a special source of groundwater must not

- Exceed 5 pCi/ℓ for ^{226}Ra or ^{228}Ra
- Exceed 5 pCi/ℓ for all alpha-emitting radionuclides except radon
- Cause a dose greater than 4 mrem to the whole body, assuming 2 ℓ/day/person consumption.

The WIPP site does not have any special sources of groundwater (WIPP Strategy, 1988).

NRC Regulations (10 CFR 60). In general, regulations of the EPA and NRC attempt to ensure that the operator, DOE, has a thorough understanding of the disposal system. The EPA regulations establish standards for protecting the general environment from off-site releases of radioactive material from a waste disposal system having multiple barriers. The NRC is responsible for assuring that a DOE disposal system for commercially generated radioactive HLW and spent nuclear fuel meets the EPA Standard.

The NRC implements the EPA Standard by incorporating it into their regulations; for example, by specifying siting criteria *(10 CFR 60.122)* that describe how to meet the "design philosophy" required in the Assurance Requirements of the EPA Standard *(40 CFR 191.14)*. Yet, the NRC also establishes minimum standards for engineered and geologic barriers of the disposal system *(10 CFR 60.113[1]* and *10 CFR 60.113[2]*, respectively) that require compliance calculations. The NRC requirements provide further assurance that the disposal system will meet the EPA requirements. The NRC stated its requirements so that they could be evaluated without many of the complexities and uncertainties associated with evaluating compliance with the EPA Containment Requirements *(48 FR 28194)*.

The combination of a minimum containment (300 yr), a maximum engineered barrier release rate (10^{-5} of inventory/yr after 10^3 yr), and a minimum groundwater travel time (10^3 yr) establishes an upper bound on the cumulative release to the accessible environment over 10^4 yr of 8.7×10^{-2} times the inventory.

Under Public Law 96-164 (1979), the WIPP is specifically exempted from regulation by the NRC. Consequently, the added requirements of NRC regulations for evaluating a geologic repository are not discussed here.

2.3 Uncertainties in Compliance Evaluation

Because of the substantial uncertainties in predicting disposal system performance for 10,000 yr, the EPA Standard requires only a reasonable expectation rather than absolute proof that a disposal system will meet the Containment Requirements. One method to provide this reasonable expectation is to

- Reduce uncertainties as much as possible with strict quality assurance procedures
- Evaluate the remaining uncertainties (preferably quantitatively).

This two-tiered approach is taken by SNLA.

The next section reviews sources of uncertainty (the long list helps the reader perceive the scope of the problem). Following sections quickly review general methods of controlling and evaluating these uncertainties. Evaluating uncertainties in the predictive results is an important reason for the complexity of the compliance evaluation, and is mentioned frequently throughout this report.

Sources of Uncertainty. Errors or uncertainty in predictions of repository performance will result from three sources (Figure 2.3) (Cranwell and Helton, 1981):

- Scenario uncertainty
- Model uncertainty
- Parameter uncertainty.

Specifically, in predicting the outcome of a scenario with a model, $F(x_1,...,x_k)$, of input parameters, $x_1,...,x_k$, either the formulation of F may be biased (model uncertainty) or $x_1,...,x_k$ may be biased (parameter uncertainty). Furthermore, because parameters $x_1,...,x_k$ have a range and distribution (parameter uncertainty), $F(x_1,...,x_k)$ (the predictions) may have a biased range and distribution (uncertainty). Finally, the scenario itself may be uncertain, scenario being defined as a sequence of events and processes that cause radionuclide release to the accessible environment. Of these sources, only parameter uncertainty is easily evaluated quantitatively as described in Chapter 4.

The modeling and parameter uncertainties for a repository are interrelated because a site must be characterized rather than designed. A site characterization begins with a crudely postulated model of the geology and hydrology, data are collected and analyzed, the model changed or refined, more data collected, etc. until the analysts are satisfied that the site has been sufficiently characterized.

Because the general categories, parameter and model uncertainty, are interrelated, classifying specific examples of uncertainty (e.g., parameter variability) is difficult and can change according to one's viewpoint. The viewpoint presented here meshes well with the data base concepts presented in Chapter 4. The following text elaborates.

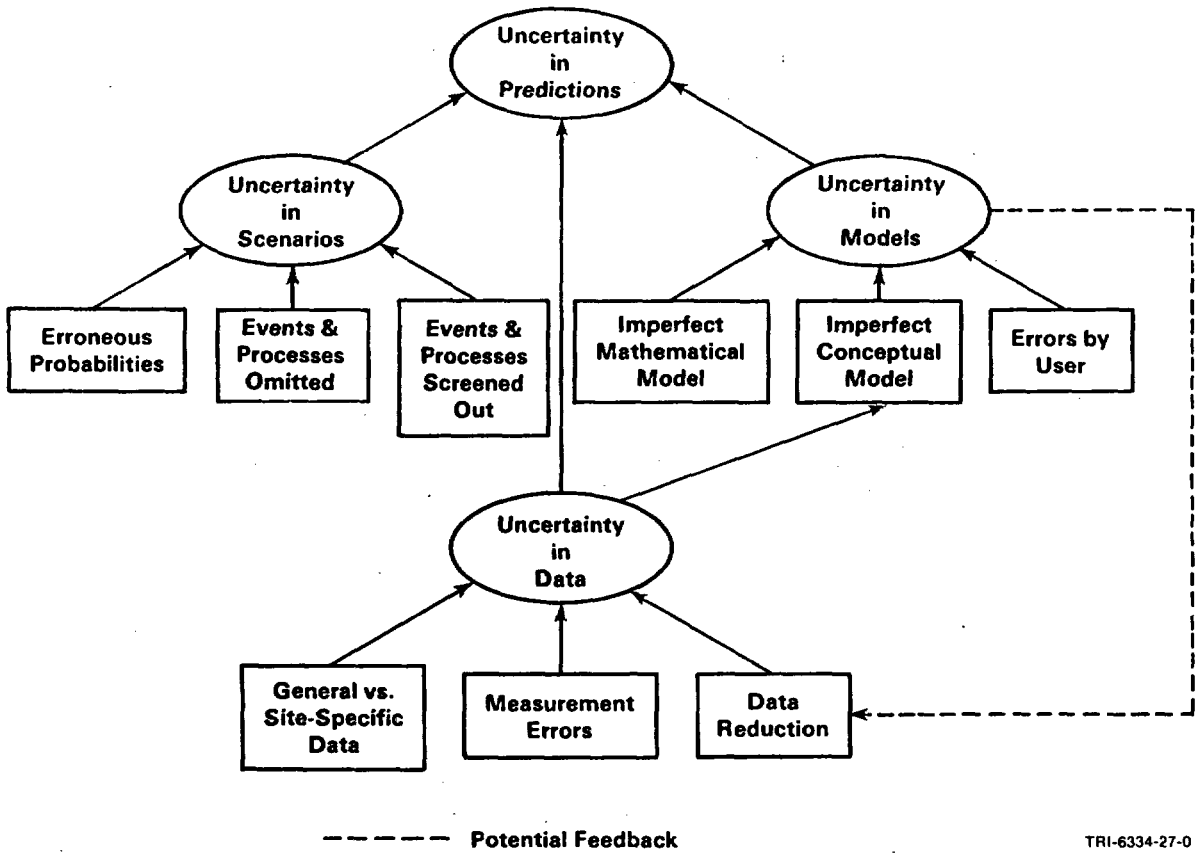

Figure 2.3 Many factors contribute to uncertainties in predictions; these factors must be controlled and evaluated.

Scenario Uncertainty. Uncertainty in the scenarios arises because (Figure 2.3)

- Important events and processes are omitted
- Important events and processes are mistakenly screened out
- Assigned probabilities for scenarios are erroneous.

Scenario uncertainty is usually controlled and reduced (external peer review) rather than systematically evaluated. A systematic method of compiling and screening scenarios increases the likelihood of including all significant scenarios. For example, collecting all conceivable scenarios and then carefully screening out physically unreasonable scenarios, low-probability scenarios, and low-consequence scenarios increases confidence of including all significant scenarios (Hunter, 1989; Hunter et al., 1986).

Assigning probabilities to scenarios is uncertain. Usually, a probability cannot be calculated, but it must be assigned by examining indirect evidence. Consequently, risk assessment policy establishes accepted procedures and degree of conservatism. The WIPP will limit and qualitatively express scenario uncertainty through external peer review.

Model Uncertainty. Modeling uncertainty originates from all four phases of model development (the conceptual model, the mathematical model, the computer model, and application) (Figure 2.4). Conceptual, mathematical, and computer models are defined as follows (Bear and Verruijt, 1987):

- A conceptual model is a set of assumptions about the physical characteristics (e.g., aquifer boundaries, material type and uniformity) and the processes (e.g., mode of flow--2D, 3D; radial, porous, or fractured media; temperature and density dependence) that affect behavior of the actual system, yet are consistent with the objectives of the model (e.g., system model vs. detailed process model)
- A mathematical model describes the conceptual model (e.g., the mass, momentum, or energy-balance equations of the property being predicted, the material constitutive equations, and the proper initial and boundary conditions)
- A computer model is the implementation (often through discretization of the mathematical equations) of the mathematical model (for this report, the computer model is also interpreted as the analytic or quasi-analytical solution that may be coded for the computer).

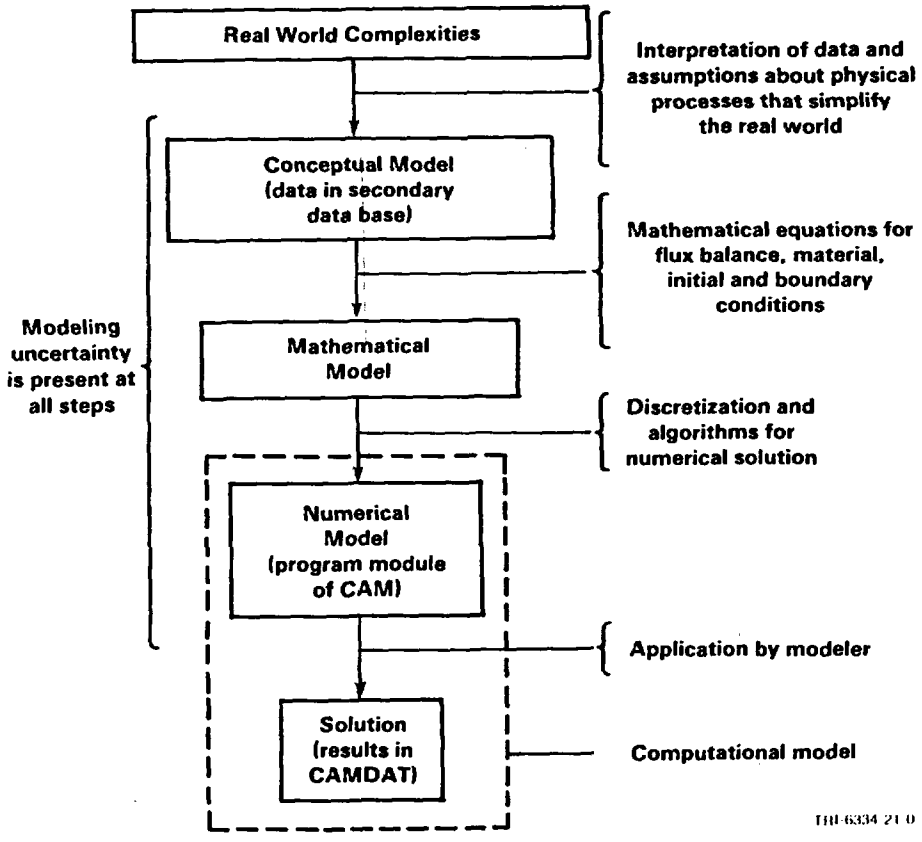

Figure 2.4 Modeling uncertainty originates from all three phases of model development.

Although not reflecting the hierarchical (and thus interdependent) nature of model development shown in Figure 2.4, specific causes for modeling errors and uncertainty include the following (Figure 2.5):

- The understanding of the phenomena (conceptual model) may be imperfect because
  - Data are misinterpreted (e.g., lab instead of field data are used, data are extrapolated or not enough data existed for interpolation, or the spatial variability of the data is poorly understood)
  - The ranges and distributions for parameters are in error
  - Alternative conceptual models are ignored (conflicting data disregarded).
- The mathematical and numerical formulation of the conceptual model (mathematical and numerical models) may be imperfect because
  - Erroneous simplifying assumptions are used (e.g., the equation for a physical process is erroneously assumed to be linear, processes are improperly coupled or decoupled, the process is inadequately approximated with lumped parameters, parameter interdependence is improperly ignored)
  - Boundary conditions are poorly understood
  - Algebraic and programming mistakes are present in the analytic, quasi-analytic, or numerical solution techniques
  - The individual codes (approximating separate physical processes) did not correctly pass results between each other.
- The analysts may introduce errors into the mathematical model because
  - The wrong data are used (even though the mathematical formulation is correct)
  - Results are misinterpreted (e.g., similar results are mixed up)
  - The mathematical model is misapplied (e.g., the analyst oversimplifies the process, improperly discretizes the problem, or fails to check for proper convergence).

As mentioned above, analysts attempt to reduce or control these modeling biases with adequate QA procedures (e.g., benchmarking, verifying, and validating models). Evaluating these biases quantitatively with uncertainty analysis is difficult.

Controlling Modeling Errors. QA ensures that the consequence analysis provides reasonable assurance that the disposal system complies with license criteria.

Because the extent of quality assurance should be commensurate with a task's complexity, importance, and risk of failure, QA must be strict for final disposal compliance assessments. However, while exploring phenomena with new models and performing experiments for preliminary compliance assessments, the QA may rely more on an analyst's expertise and scientific scrutiny by peers than on procedural methods.

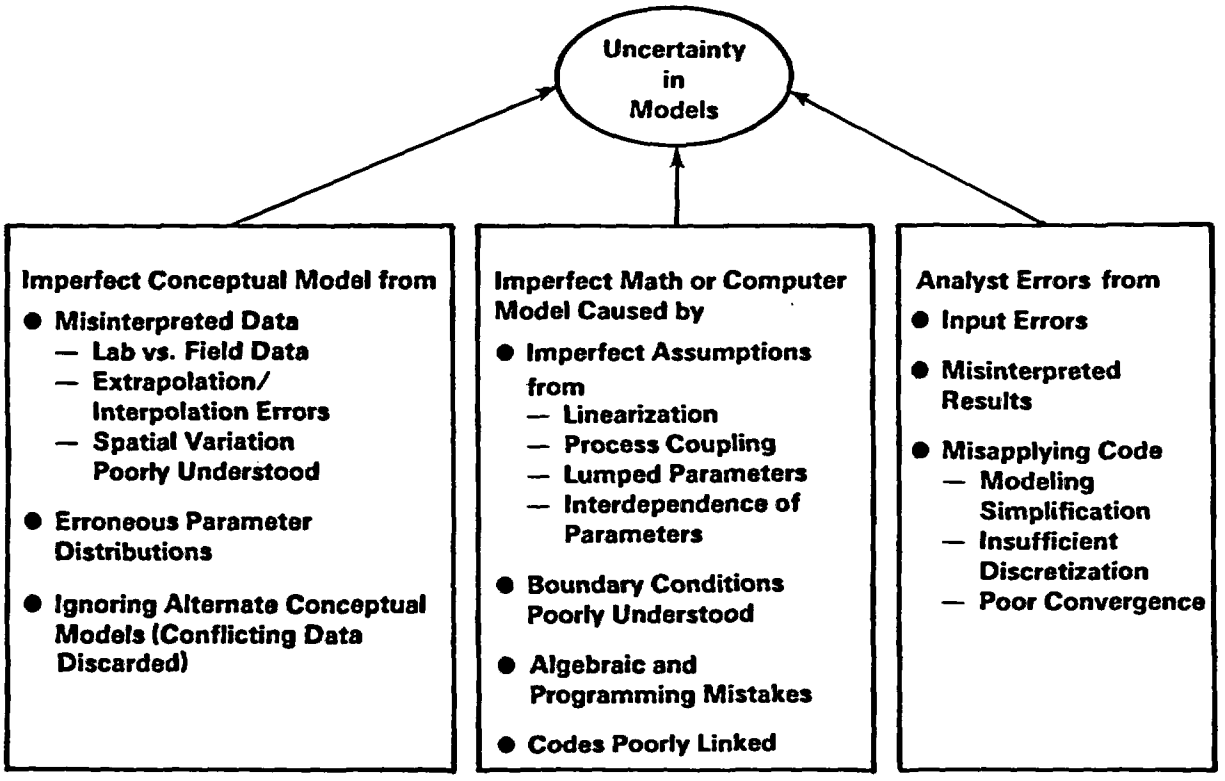

Figure 2.5 User errors, imperfect conceptual models, and imperfect mathematical models contribute to modeling uncertainty.

The best management strategy is to build in quality. First, the analyst and tools used by the analyst should be capable of providing the quality of work expected. Second, design and analysis should be a chain of tasks, interrupted frequently by peer reviews. The following text discusses reduction of uncertainties using two convenient and interrelated categories:

- Quality assurance of tools and techniques used (Software QA)
- Quality assurance of analysts' work (Analyst QA).

Software QA. For the analyst, the usual tools are computer software. Software provided to the analyst should be capable of delivering the quality of work expected. Each analyst on a large project cannot adequately assure software quality.

Software QA requires user manuals to describe the type of problem and equations that a code is able to solve, the method of solution, and the required input. Output listings must properly identify the code, date, and version number. Comments within the software should include a brief description of origin, variables, names of authors, and the history of modifications. The documents should also include test or benchmark problems verifying that the software performs as claimed (code verification).

The user also needs a reference or filing system to keep track of current versions of software and necessary documents. The reference system provides a secure place to store current and archived listings

of software and manuals. Such a filing system ensures that people use current versions of all software and can retrieve old software to trace past work. The system can be stored on the computer or in a reference library, provided that the documents, listings, and history of modifications remain complete.

The data transfer techniques described in this report are a very important tool of the analyst and ensure that a quality analysis is possible (Chapters 5 and 6).

Analyst QA. Software QA cannot assure the quality of problem data or modifications to software, or ensure the proper use of the software. Quality assurance of the overall design and analysis is needed. The engineer's or scientist's expertise ensures that these details are correct (necessary to achieve high caliber work), determining to a certain extent how well these broader issues are addressed.

Management supplements this expertise by providing a framework for quality analyses, placing some controls on the design and analysis process. Again, documentation, which allows another person to understand the approach and the software used, and to check the work, is a preliminary step.

Specifying objectives and adequate planning are additional quality controls. Still another quality control is peer review. Although the burden of ensuring correctness is not passed on to the reviewer, the review can help the analyst achieve high-quality work.

More stringent controls are possible, such as developing procedural manuals and carefully assembling data bases with strict QA of data entered. A suggested form for a data base of measured data, called a primary data base, is discussed in Chapter 5.

Model Validation. To reduce modeling uncertainty, analysts attempt to remove biases by validating the model against several independent observations, using site-specific parameters. Because an analyst is using site-specific parameters, model validation checks the conceptual model, as well as the mathematical and computer model.

Ideally, testing should require that the parameters vary over their entire expected range,excepting time. For practical purposes, the model is valid when testing shows that the model predicts observations accurately. Because subjective criteria are used to assess the validity of a model (e.g., reasonable lengths of time, costs, and accuracy), model validation has no definitive endpoints; only a general consensus can be reached.

Evaluating Modeling Uncertainty. If a model cannot be completely validated, evaluating modeling uncertainty centers around using alternate conceptual and mathematical models. An alternate conceptual model might involve a difficult model change (still supported by the available data) from porous media flow to fractured media flow or might involve an easy model change such as changing a formation from permeable to impermeable (note that the latter alternate conceptual model could be classified as parameter uncertainty, but the distinction is not entirely clear).

Use of alternative conceptual models is limited by time and resources; thus, modeling uncertainty may need to be evaluated more qualitatively through expert opinion or, as discussed later, by purposefully increasing parameter uncertainty.

Parameter Uncertainty. Causes for parameter bias or uncertainty include (Figure 2.6):

- Using general versus site-specific data
  - lab versus field data
  - indirect observations (e.g., misinterpreted natural analogs)
  - use of inappropriate literature data (which may have measurement or data reduction uncertainty)
- Measurement errors caused by
  - sampling bias from insufficient or poorly spaced samples
  - measurement conditions not representative of an operating repository
  - measurement technique misapplied
- Data reduction errors (improper parameter estimation) caused by
  - spatial variability of parameters
  - interpreting experiments using a model inconsistent with repository conceptual model
  - misinterpreting the interdependence of parameters.

Spatial parameter variability, is a distinct problem for deterministic models which use a single value for each parameter to produce a single prediction. Consequently, the natural variation of the parameter (due to representing a distributed property as a lumped constant) and the random measurement and sampling errors are unaccounted for.

Similarly to modeling uncertainty, analysts attempt to remove or control these data biases with adequate QA. Analysts also attempt to evaluate these biases, both qualitatively and quantitatively, with uncertainty analysis.

Controlling and Evaluating Parameter Uncertainty. Whenever predictions are made for conditions different from those for which the models and their data bases were developed, improper parameter estimation (and possibly model bias) can occur. Again, model validation can help alleviate problems.

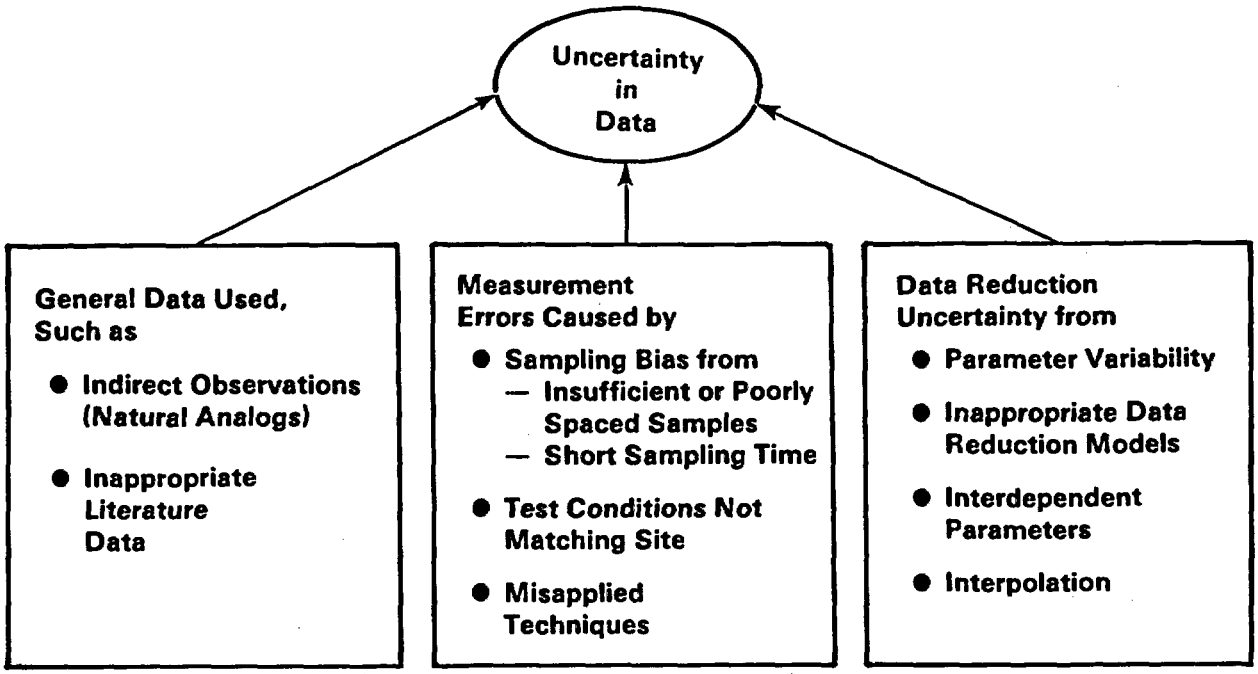

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Figure 2.6 Measurement errors, data reduction, and use of general data contribute to data uncertainty.

If the mathematical model of the system is unbiased, a frequency distribution of parameter values can be used to estimate the parameter uncertainty. An analyst evaluates parameter uncertainty either by incorporating parameter uncertainty directly when formulating the problem (stochastic approach) or by combining a Monte Carlo sampling with a deterministic formulation of the problem. SNLA's compliance assessment methodology emphasizes the deterministic formulation; thus, in Chapter 3 parameter uncertainty is discussed primarily from this latter point of view. The results of this uncertainty analysis are assembled into probability distribution for comparison to the EPA Standard.

3. SNLA Compliance Assessment Methodology

This chapter briefly describes a method for assessing the regulatory compliance of a repository. Many of the topics related to uncertainty are elaborated upon. Although the concepts were first developed for nuclear reactor safety studies at SNLA and elsewhere, SNLA was instrumental in combining the concepts for evaluating repository performance (NEA, 1988; Campbell and Cranwell, 1988; Cranwell et al., 1987).

If you have had an introduction to this subject, you could skip to Chapter 4, which discusses how these technical requirements affect data flow. Otherwise, use Chapter 3 as a brief introduction to methods for evaluating repository compliance. Hunter et al. (1986) also provide an explanation, along with an example problem.

Only after becoming involved with all the required data collection and modeling does one fully appreciate the magnitude of the EPA Standard requirements for a compliance assessment.

3.1 Tasks in Methodology

To perform probabilistic risk assessments, one must evaluate both the probabilities and consequences of events and processes that could transport contaminants from a waste site to a specific target. The five tasks in assessments usually are (NEA, 1988; Helton et al., 1988; Cranwell et al., 1987):

1. Disposal system (waste properties, site characteristics, and facility design) and regional area characterization (i.e., system characterization)
2. Scenario development (event and process identification, screening, scenario construction, further screening, and estimation of probabilities) (procedure similar to accident progression analysis in nuclear reactor PRAs)
3. Source-term and consequence modeling; i.e., systems analysis (sometimes treated as two separate tasks)
4. Sensitivity/uncertainty analysis
5. Comparison with government regulations.

The first two tasks establish the conceptual model of the disposal system and surrounding region for each significant scenario (i.e., the complete description consistent with the purpose of the analysis, based on an analyst's interpretation of available data). The third task consists of mathematically modeling the conceptual model.

To complete the fourth and fifth tasks, it is necessary to integrate the third task into an overall, coherent analysis. Several criteria must be met. The analysis must

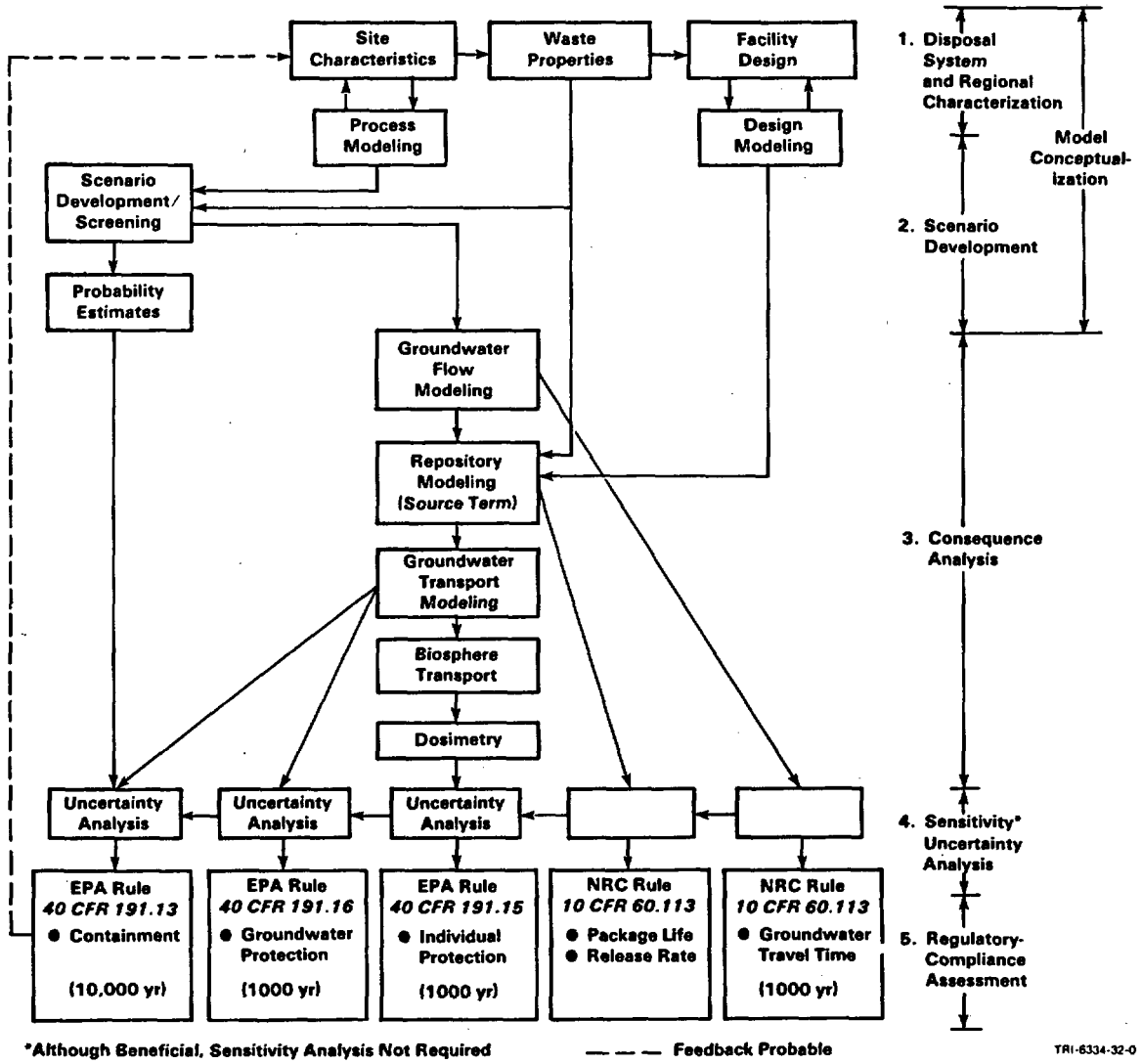

Figure 3.1 SNLA's method for assessing repository compliance involves five tasks.

- Examine a large number of intermediate and final results
- Incorporate quality assurance procedures
- Accommodate large uncertainties in input and output
- Permit both uncertainty and sensitivity analysis even when significant nonlinearities occur within modules
- Be computationally fast.

The first two criteria are the main points of discussion of this report; however, the latter four are still very influential in the design of the system. SNLA's approach is to

- Modularize the tasks
- Use Monte Carlo techniques with efficient Latin hypercube sampling (LHS) to propagate uncertainties
- Use fast-running mathematical modules or computational subdomains of the disposal system where appropriate
- Provide well defined interfaces between individual parts of the analysis
- Automate the overall analysis as much as possible.

Concerning the first feature, SNLA's modular approach to risk assessment is shown in Figure 3.1. The five tasks of the methodology are represented by the various modular blocks. This modular approach has several advantages:

- The analyst, by examining intermediate results, gains insight into physical processes and important parameters affecting risk
- The analyst can use intermediate results directly in screening scenarios and performing sensitivity analysis
- The analyst can modify the methodology, if necessary, to allow for site- and design-specific characteristics.

Making the procedure conceptually modular is the first step. An important second step is to create a data flow structure so that the procedure is modular in practice. A method for doing that is presented in Chapter 5.

The following sections discuss the five basic tasks of a compliance assessment in more detail and describe how SNLA combines them into a coherent analysis.

3.2 Task 1: Disposal System and Surrounding Area Characterization

System Components to Characterize. The first task is to describe the disposal system and the surrounding area, which requires knowing the characteristics of

- The engineered barrier (waste properties and packaging, waste placement and backfill, and facility design)
- The natural barrier (site geology, hydrology, and geochemistry)
- Geologic setting (regional geology and hydrology).

Tyler et al. (1988) and Lappin (1988) summarize the extensive characterization at the WIPP of the engineered barrier and site, respectively.

The natural geologic barrier determines the design of the engineered barrier because unlike the natural barrier, the waste behavior and facility design can be controlled to various degrees; for example, waste behavior can be modified by reducing volumes, adding backfill, or adding chemical getters to change the structural and geochemical response of the room.

Iteration of Site Characterization. The site geology is not designed, and a fundamental difference exists between specifying and/or controlling a property and exploring to deduce that property. The latter is a time-consuming, iterative process subject to more errors. The iterations in characterization are

- Nonintrusive site exploration
- Preliminary interpretation and simple analysis
- Extensive site exploration (e.g., exploratory shaft; regional hydrologic data collection)
- Analysis and interpretation
- Follow-on data collection and analysis.

Enlargement of this process to include iterations within the compliance assessment methodology is discussed later.

This simple procedure of progressively collecting more detailed data after interpretation helps assure that the site evaluation is reasonably well directed and that resources are spent on the most important questions. Although this approach is the best, there are still hazards in geologic evaluations. In general, the reasons for exploratory programs failing to develop an accurate conceptual model in the past have included (Osterberg, 1979)

- Failure to carefully evaluate data which contradict an initial hypothesis or preconceived notion of the site
- Failure to use all information on site (such as general geologic processes), even though simple or obvious
- Failure of participants in widely varying organizations to communicate (specifically, to discuss the goals of the exploratory program)
- Loss of "corporate memory" on lengthy projects because of personnel turnover.

The above difficulties in site characterization and how the responsible agency addresses them are the subject of the site characterization plans (SCPs) required by *10 CFR 60* (e.g., the Yucca Mountain Project [YMP] SCP, 1988) or WIPP Yearly Program Plans and WIPP Compliance Plans (WIPP Strategy, 1988; Bertram-Howery and Hunter, eds, 1989). The SCP and experiment plans must keep the compliance assessment as the central theme, using the information provided by the compliance assessment to design a licensable waste repository. Much of the site characterization of WIPP was conducted prior to promulgation of the EPA Standard, but is directly applicable to compliance assessment needs.

Important Information to Gather. The site characterization process must gather data

- To explore the importance of various phenomena and to develop models/codes (research)
- To provide data for use in the compliance assessment.

Because the two characterization purposes differ, the data required can differ. The data for the characterization establish existing conditions. The data for the compliance assessment establish initial conditions for projecting 10,000 yr into the future and predicting potentially disrupting events. In

general, greater detail is needed for demonstrating an understanding; while greater breadth of types of data is needed for compliance assessments. However, many exceptions exist. Furthermore, the breadth of information collected for the compliance assessment can, in turn, produce a more thorough understanding of the site.

Several processes may be important for characterizing a disposal system. For the site geology, factors that influence groundwater flow and radionuclide transport will be important; these factors include evaluating flow conditions around the site (boundary conditions, porous or fractured media behavior, whether steady-state or transient conditions prevail, and saturated or unsaturated flow). For radionuclide transport, these factors include, in addition to those mentioned for groundwater, the retardation and dispersion of radionuclides.

For the engineered barrier, factors that influence the source term and close-in mobilization will be important. Such factors include the initial inventory of radionuclides, their half-lives, their solubility limits, water inflow (accounting for backfill and seals), susceptibility to leaching, gas generation from microbial decay, radiolysis, or radiological decay (accounting for any gas getters in the backfill), and the time, temperature, and chemical dependency of these processes.

Sources of parameter data include laboratory measurements, field measurements and interpretation of geologic and hydrologic records at the site, interpretation of natural analogs, and literature and expert opinion. The analyst uses the first two primary data sources (stored in a primary data base), along with the latter two sources to develop a conceptual model of the disposal system (stored in a secondary data base) for each scenario analyzed.

3.3 Task 2: Scenario Development

Although system characterization is important to an understanding from which to develop conceptual models of the repository, scenario development is equally important for showing regulatory compliance. A scenario is defined herein as a sequence of events and processes, either singly or in combination, that could contribute to radionuclide release into the accessible environment (Cranwell et al., 1987). The systematic procedure for developing and selecting scenarios at WIPP (Cranwell et al., 1988) (Figure 3.2)

1. Identifies all events and processes important to long-term isolation of radioactive waste in deep geologic formations through literature searches and expert opinion.
2. Classifies events and processes as to
   - Manner of movement from waste package
   - Whether influence is on transport through waste package or barriers
   - Whether event is anticipated or unanticipated *(10 CFR 61)*.
3. Establishes probability ranges for events and processes (for screening in Step 4) by
   - Determining frequencies from existing data
   - Modeling the event either stochastically or deterministically with Monte Carlo sampling

- Subjectively evaluating with expert opinion (highly formalized).

4. Screens events and processes in order of importance by (Figure 3.3)
   - Physical reasonableness
   - Simple estimates of potential consequences
   - Probability of events and processes (e.g., disregarding events with probabilities less than 10^{-8}/yr [*40 CFR 191*])
   - Regulatory guidance in Appendix B of *40 CFR 191* (e.g., maximum number of borehole/km^2 to use for human intrustion scenarios).
5. Combines events and processes to form mutually exclusive scenarios that can be analyzed.
6. Establishes probabilities for scenarios for screening in Step 7 and later for compliance evaluations, using techniques similar to Step 3.
7. Develops a final scenario list by
   - Screening scenarios using the same criteria used for Step 4
   - Pooling "similar" scenarios to form a single scenario.

For the WIPP, most important natural processes at the site were identified during site characterization. However, the importance of some phenomena to the compliance assessment was only recognized after scenario development. For example, the importance of predicting the extent of salt encasement of the waste (controlled by the amount of brine inflow, gas generation, and salt creep) for the human intrusion scenario was only recognized after scenario development.

For the WIPP, events retained for scenario development included (Hunter, 1989) effects of a pressurized brine pocket beneath the repository, climatic change, dissolution of rock adjacent to the repository, drilling into the repository, groundwater flow, effects of mining for resources, seal failure, subsidence of overlaying rock into the repository, and waste-rock interaction. The scenarios from these events can be collected into three major groups based on similarity of modeling approach: (1) the human-intrusion scenario group, (2) the climatic change and/or shaft leakage group, and (3) the undisturbed scenario.

Initially, 110 scenarios describing possible pathways for waste release into the accessible environment were developed. Initial screening reduced this to 76 scenarios (Hunter, 1989). After final screening with bounding calculations, about 10 probably will remain--a manageable number to evaluate thoroughly.

3.4 Task 3: Consequence Modeling

Modeling Components. Besides system characterization, a major portion of the methodology consists of simulating physical processes to estimate the amount of radionuclides released to the accessible environment (consequence modeling). The modeling system consists of four parts:

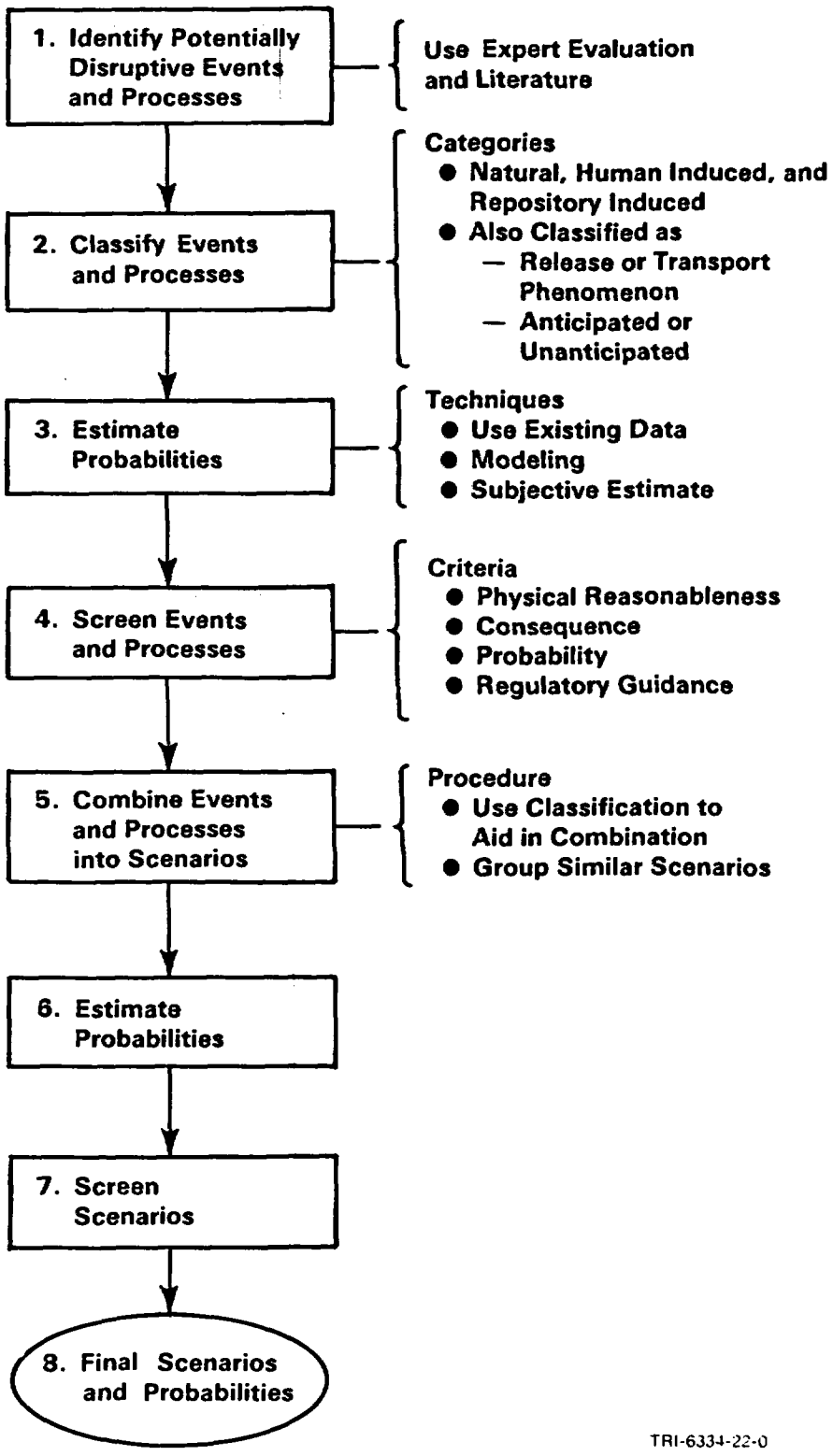

Figure 3.2 Scenario development involves event and process identification, screening, scenario construction, and further screening.

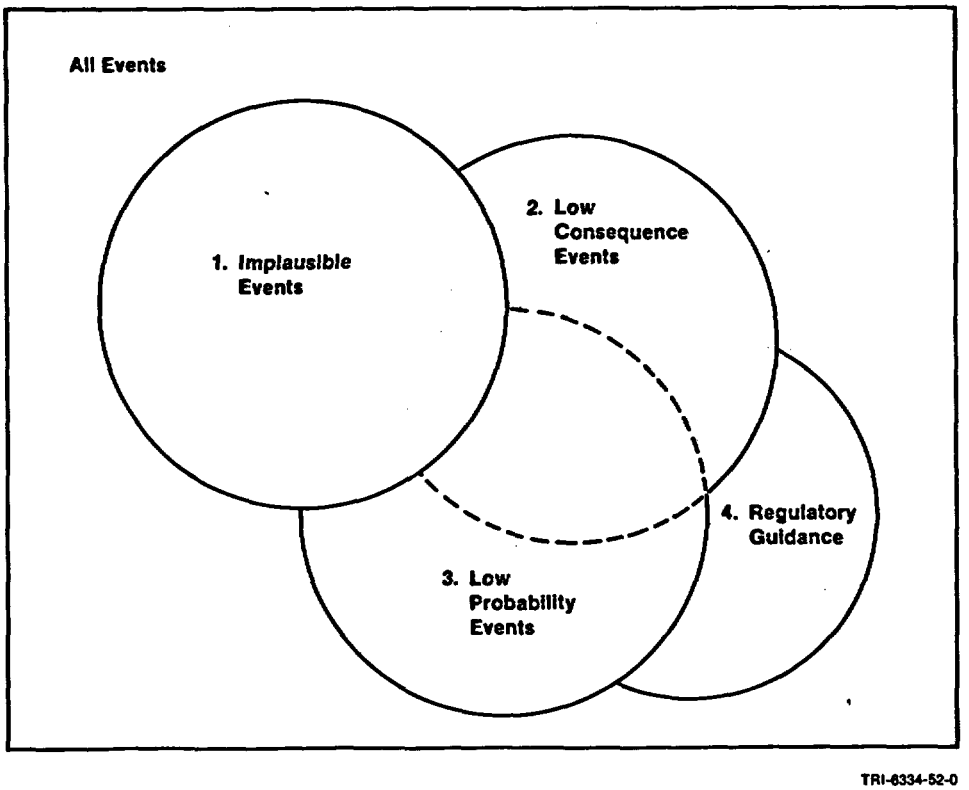

Figure 3.3 Four general criteria exist for screening scenarios.

- Groundwater flow
- Source-term calculation
- Radionuclide transport in the geosphere and biosphere
- Dosimetry and health effects.

Radionuclide transport uses two distinct modules for geosphere and biosphere transport. Likewise, two distinct modules are often used for groundwater flow, the first process listed. The two scales are used to make the consequence analysis more tractable and are discussed in Chapter 4.

Consequently, the six typical computer modules of the consequence assessment are

- Regional groundwater flow module
- Local groundwater flow module
- Repository/shaft (including source-term, room, panel seal, drift, and drift seal) module
- Lithosphere (e.g., ground water) radionuclide transport module

- Surface-water, atmosphere, and biological radionuclide transport (succinctly labeled biosphere transport) module
- Dosimetry module.

Because of the strong influence upon data flow, these modules are discussed in greater detail in later chapters; however, a cursory explanation of their purpose follows. The regional groundwater flow module predicts groundwater flow patterns in a region around the controlled area of the repository. It extends to natural groundwater boundaries where possible. Boundary conditions for the next smaller scale model, the local groundwater flow module, are calculated from the regional flow fields. The regional flow conditions then set boundary conditions upon the smaller scale model, the local groundwater flow model. Flow patterns in the controlled area are calculated by the local groundwater flow module. Compliance with the NRC groundwater travel time requirement can then be evaluated.

Next, the local model sets boundary conditions for the repository model for scenarios in which groundwater enters the repository. After this stage, compliance with the NRC engineered barrier requirements can be evaluated. The repository model establishes the source-term for the groundwater transport module. Following the transport calculations, compliance with the EPA containment and groundwater protection requirements can be evaluated.

The last two modules, biosphere transport and dosimetry, are used to evaluate compliance with the EPA Individual or Special Groundwater Protection Requirements.

Linkage of the modules, including typical data requirements and data transferred, are shown in Figure 3.4.

Component and Data Selection. To apply each of the models used in a consequence analysis, an analyst goes through three steps (Cranwell et al., 1987):

- Selecting/developing codes suitable for modeling the physical events and processes making up the various scenarios
- Selecting data for code input and selecting parameters to vary for uncertainty analysis
- Accurately linking and running the computer models to predict potential outcomes for each scenario.

Code Selection or Development for Compliance Assessments. During Task 1, disposal-system characterization, modeling is necessary for characterizing and conceptualizing the site (to aid in the current understanding of the site). Some detailed numerical models explore the interaction of various processes and other, simple analytic models assess whether certain processes are important to the disposal system (e.g., assessing the importance of fractured media flow [Beauheim, 1987; Tomasko and Jensen, 1987]). Specifically, the codes are selected or developed for two primary purposes: (1) to determine ("reduce") hydrologic and material parameters from the observed data and (2) to attempt to reproduce the observed data (e.g., pump drawdowns) understanding of geology/hydrology/geochemistry processes of the geologic barrier.

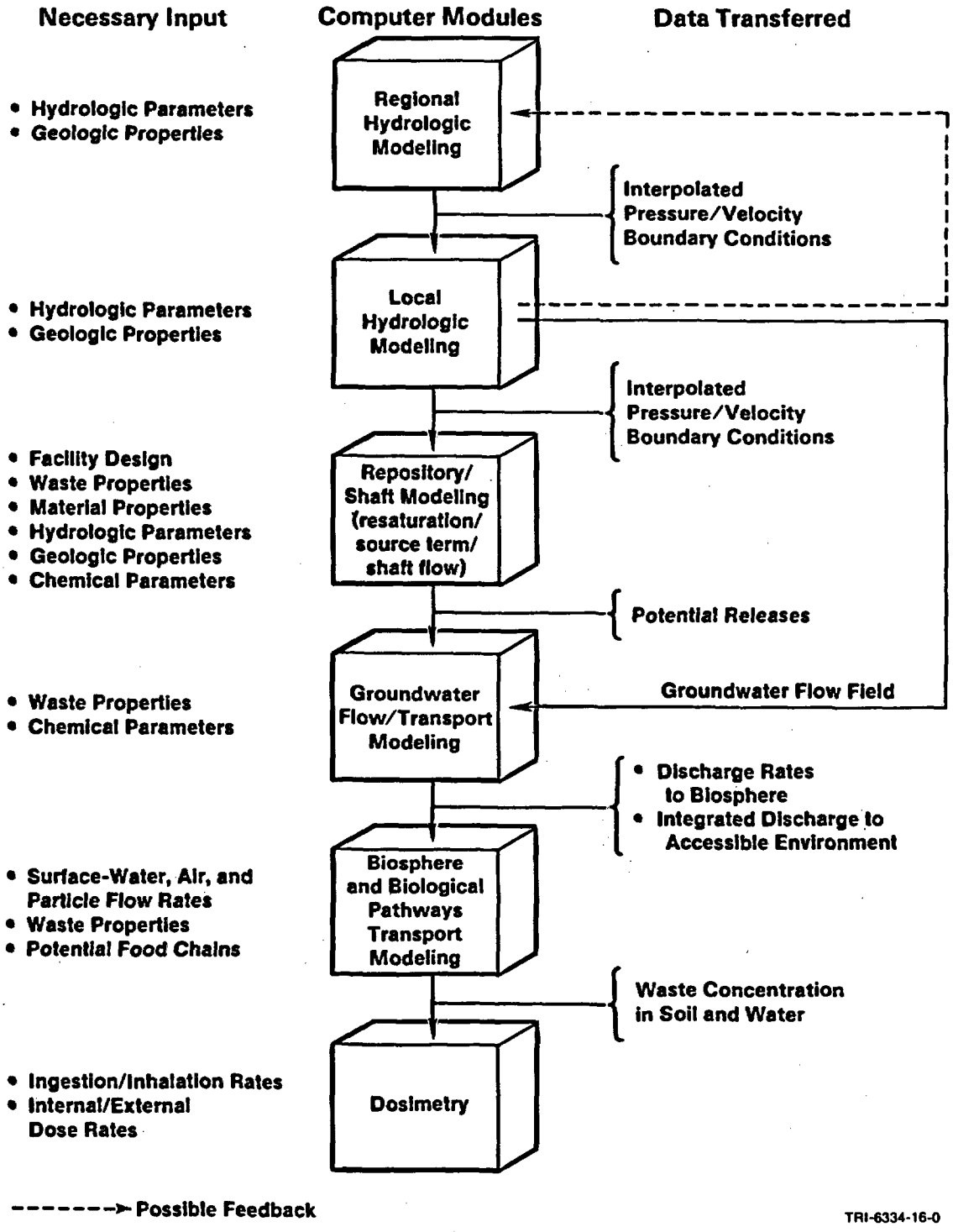

Figure 3.4 Six model categories were used in assessing the consequence of a scenario in the WIPP (after Cranwell et al., 1987).

However, the purpose of modeling for consequence analysis differs from the usual scope of modeling for site characterization. Modeling in conjunction with consequence analysis simulates conditions 10,000 yr into the future, while accounting for uncertainty contained in parameters of the computational model derived from site characterization. Consequently, while models/codes used to reduce or reproduce data can be detailed and slow-running, models/codes used to predict consequences while propagating uncertainty must optimize between two choices:

- Physical modeling realism (which affects credibility)
- Fast-running for propagating uncertainty using Monte Carlo sampling (which affects tractability of the performance evaluation).

To elaborate, although the computational burden of any one module must remain small so that computations for the overall analysis remain feasible, reducing the complex physical processes (e.g., salt creep, waste compaction, and brine resaturation) defies easy simplification.

Further, the list of scenarios may require selection or development of codes not specifically required for characterization (e.g., radionuclide transport). In addition, because of the large variety of disciplines involved, individual analysts may focus on their specific areas or use techniques that are not compatible for questions concerning the system as a whole. Finally, the complex process of compliance evaluation requires the development of efficient data flow (e.g., the computational data base discussed in this report). Herein lies the challenge in developing a credible case that a nuclear waste repository complies with regulations.

Consequently, although codes were selected and used for data reduction and reproduction, the typical three-step process of identifying models needed, selecting codes, and optimizing their computational efficiency must be repeated for consequence analysis.

Once selected, an important requirement for codes is that they be verified, and the conceptual and computational models validated to the extent possible, using site-specific data to limit uncertainty. Furthermore, the serially coupled system of codes must also be verified and validated--a lengthy process.

Selecting Data Input. Selecting values for the numerous parameters listed in Figure 3.4 is arduous. Typically, the deterministic model approximates continuously varying rock properties with lumped parameters. Uncertainties in the best estimate of a lumped parameter are handled by Monte Carlo sampling; however, ranges and types of distributions must be specified. Correlations with other lumped parameters may also exist and must be specified. Even with these correlations and plausible distributions and ranges, certain combinations of parameters may still produce nonsensical results, which place further constraints on permissible parameter values.

Selecting parameter values, a part of model conceptualization, is begun during site characterization. For example, statistically significant changes in parameter values may be used to identify subtle changes or trends within stratigraphic layers of a geologic formation. However, parameter selection cannot be completed until all conceptual and derived mathematical models are selected.

Accurately Linking and Running the Codes. Ensuring that the output from one code is compatible with the required input for the next code (linking the codes) is not trivial. The process of linking and running the codes to accurately propagate intermediate results is the major topic of this report and is discussed in Chapters 4 and 5.

3.5 Task 4: Sensitivity/Uncertainty Analysis

With sensitivity/uncertainty analysis, an analyst evaluates the potential variation of parameters and their relative importance to the results. A consequence module is a function, $F_1(x_1,...,x_n)$, of variables $x_1,...,x_n$. Because $x_1,...,x_n$ have ranges and distributions, $F_1(x_1,...,x_n)$ will also have a range and distribution. Uncertainty analysis involves determining properties of the distribution of F_1. These properties include the distribution, expected value, and variance of F_1. Sensitivity analysis involves determining the importance of an individual, x_n, in influencing F_1 and its uncertainty.

The above function, F_1, represents one consequence module of the compliance assessment. The predicted release for radionuclide i and sample run k, q_{i_k}, is a function of the many modules, F_ℓ, of the CAM:

$$q_{i_k} = F_3\{z_1,...,z_q, F_2[y_1,...,y_p, F_1(x_1,...,x_n)]\} \qquad [3.1]$$

where

F_ℓ = ℓth consequence module (three modules assumed in [3.1])

x_n, y_p, z_q = variable of consequence modules F_ℓ ; some variables may be identical

q_{i_k} = release at time t for radionuclide i for sample run k.

Evaluating the system-wide importance of the individual variables ($x_1,...,x_p$, $y_1,...,y_p$, and $z_1,...,z_q$) influencing the distribution of q_{i_k} (uncertainty expressed by different sample runs, k) is challenging. The predicted release, q_{i_k}, is used in calculating the summed normalized release, $\hat{R}_k$, described under Task 5, in Section 3.6. The distribution of q_{i_k} directly translates into a distribution of $\hat{R}_k$, from which comparisons are ultimately made with the EPA Standards.

Uncertainty Analysis. An analyst evaluates uncertainty either by incorporating variable uncertainty directly when formulating the problem (stochastic approach) or by using a deterministic formulation and incorporating variable uncertainty indirectly as described below. Both methods are useful. SNLA chose to use a primarily deterministic approach and to depend on stochastic analysis if collaborative analysis was required because

- Important physical phenomena can change between scenarios, which can require model changes
- More deterministic models at various levels of detail are available for the major phenomena than stochastic models are (stochastic modeling, still in research stage, has no validated models).

Three techniques appropriate for propagating and analyzing uncertainty in predictions from deterministic, complex models are

- Differential analysis using normalized partial derivatives of parameters (Frank, 1978) and often implemented by the adjoint procedure (Oblow et al., 1986; Pin et al., 1986)
- Development of surrogate analytic expressions for results (response surface methodology) or models (e.g., Fourier amplitude test) (McRae, 1982)
- Monte Carlo analysis (sampling from the distribution of input parameters to generate a distribution of output) (McKay et al., 1979; Iman and Conover, 1980; Iman et al., 1981; Rubinstein, 1981).

Comparative discussions of these techniques are found in various reviews (e.g., Iman and Helton, 1988; Iman and Helton, 1985).

Although other methods do exist, they are generally inappropriate for handling uncertainty problems of the type encountered with complex models. For example, propagating optimistic, central, and pessimistic assumptions is inappropriate for the rigorous EPA standards. The Maximus methodology is limited to propagating binomial and Poisson distributions, and Kalman filtering requires past observations for adjusting predicted behavior from a model (Helton et al., 1988).

Of the three appropriate techniques, SNLA chose Monte Carlo analysis for four major reasons. First, Monte Carlo analysis creates a mapping from input to output that can be studied by a variety of techniques (e.g., scatterplots, distribution functions, regression analysis, partial correlation analysis). This mapping is well-defined for any input vector if the input parameter space is properly sampled. Unlike differential analysis and response surface methodology, this mapping does not smooth and obscure discontinuities and transitions between regimes of behavior.

Second, Monte Carlo analysis can accommodate large uncertainties and discontinuities. Although the analysis is complicated by these factors, it is superior to other techniques when large uncertainties and discontinuities exist (Helton et al., 1988).

Third, Monte Carlo analysis can propagate and analyze uncertainty through several linked modules.

Finally, Monte Carlo sampling can include variables with wide ranges and incorporate correlations between variables.

Although the Monte Carlo method was chosen as the primary method of propagating uncertainty and analyzing parameter sensitivity through the linked modules, this choice does not preclude the use of other techniques such as differential analysis or even parameter variation studies when examining individual modules.

Because Monte Carlo sampling was chosen for propagating and analyzing uncertainty, computational costs are important. Costs are controlled by

- Embedding models
- Using fast-running codes as surrogates for more detailed codes when appropriate.

Another technique for controlling costs is collecting and aggregating intermediate results to reduce the quantity of results from calculations (Helton et al., 1988). Although useful for event trees when analyzing nuclear power plants, its usefulness for geologic repositories is limited.

Sensitivity Analysis. As defined, sensitivity analysis evaluates the importance of a parameter on the variation in the result. However, two different measures of variable importance exist.

Definition of Importance. Although not used in SNLA's performance evaluation procedure, differential analysis is a convenient method for defining two frequently used measures of importance. Specifically, in differential analysis the model is approximated by a Taylor series:

$$q \simeq q(X_0) + \Sigma_n \frac{\partial q(X_0)}{\partial x_n} \{x_n - x_{n0}\} \qquad [3.2]$$

where

q = predicted release

X = vector of variable values, x_n

X_0 = vector of "base case" variable values, x_{n0}.

Because the partial derivatives of [3.2] are dependent on units, they are typically normalized to either

$$\frac{\partial q(X_0)}{\partial x_n} \frac{x_{n0}}{q(X_0)} \qquad [3.3]$$

or

$$\frac{\partial q(X_0)}{\partial x_n} \frac{S(x_n)}{S(q)} \qquad [3.4]$$

where

$S(x_n)$ = standard deviation of x_n distribution

$S(q)$ = standard deviation of q distribution.

Depending on the analyst's preference, an ordering of the absolute values of either [3.3] or [3.4] can be used to measure and rank variable importance, I_n. Using [3.3],

$$I_n = \left| c_n \frac{x_{n0}}{q(x_0)} \right| \quad . \qquad [3.5]$$

Otherwise, using [3.4],

$$I_n = \left| c_n \frac{S(x_n)}{S(q)} \right| \qquad [3.6]$$

where

$$c_n = \frac{\partial q(X_0)}{\partial x_n} \quad .$$

Equation [3.5] ranks variable importance based on the effects of equal percentage changes from the base case values x_{nO} (the traditional sensitivity analysis introduced by Tomovic, (1963). The normalization in [3.6] ranks variable importance based on the effects of equal percentage changes of the standard deviation, $S(x_n)$. Hence, [3.6] folds in the likelihood that a variable, x_n, will vary enough to potentially influence the result, q, while [3.5] does not.

The normalization expressed by [3.6] is especially useful because, conceptually, [3.6] is similar to standardized regression coefficients (SRCs):

$$I_i = \left| b_i \frac{S(x_n)}{S(q)} \right| \qquad [3.7]$$

where b_i denotes a model regression constant (Helton et al., 1986) ($b_n = c_n$ for linear models).

The absolute values of SRCs (and the mathematically related partial correlation coefficients) are frequently used for ranking variable importance when complex computer codes describe the model (numerical sensitivity analysis). The method involves constructing a regression model between the variables and the observed response, q (Iman and Helton, 1985), in conjunction with a Monte Carlo approach (such as Latin hypercube sampling [LHS] with constrained pairing [Iman and Conover, 1980]).

The measure of importance expressed by Equation [3.7] is very useful for environmental models, where variables may vary over several orders of magnitude, because an important purpose of a sensitivity analysis is to allocate data collection resources towards those variables that most influence R, based on what is already known about the site. Equation [3.7] is more useful than [3.6] because b_i describes the trend of a more linear function, q, over several orders of magnitude in contrast to c_i, the slope of the function at one point, in particular. When a variable is precisely known, SNLA may not want to allocate more resources to evaluate it.

Two Levels of Sensitivity Analysis. Two steps can occur with sensitivity analysis; the information gleaned at each step differs. An analyst may perform sensitivity analysis on

- Individual module components--
- The system as a whole.

Evaluating variable importance of an individual component allows an analyst to more fully understand an individual code and the importance of the physical processes it represents. Evaluating variable

importance of the entire system allows an analyst to gain insight about the system. Both are important. Sensitivity analysis of individual components is important for developing a module from detailed phenomenological models useful for the compliance assessment.

Likewise, system-wide sensitivity analysis is useful for evaluating the relative importance of system components. The results may permit use of simple, fast-running components in the uncertainty analysis, thereby making the uncertainty analysis more tractable. Furthermore, this approach to evaluating component importance is more easily defended in comparison to "expert opinion" whenever risk assessment policy decisions are questioned by other agencies or the courts.

Nonlinear or even discontinuous behavior greatly complicates the sensitivity studies; consequently, sometimes only a measure of insight rather than complete understanding is obtained. Furthermore, when evaluating the system as a whole, studies must be carefully planned (e.g., judiciously choosing which parameters to examine) to provide insightful results. Otherwise, the sensitivity analysis may only provide intuitively obvious results--an admonition applicable to all studies on large systems, mathematical or otherwise.

Unlike uncertainty analysis, sensitivity analysis is not a requirement of the regulations and, thus, is not a part of the final analysis. Sensitivity analysis is a technique to gain understanding and insight about the system. Hence, its primary usefulness is in the early phases of an assessment to help produce necessary understanding and allocate resources to develop a credible compliance assessment (Konikow, 1978).

3.6 Task 5: Compliance Evaluation

Although described as a distinct task in compliance assessments, the fifth task, compliance evaluation, occurs after various steps of consequence analysis. For instance, an analyst can assess compliance with the NRC 1000-yr, groundwater travel time requirement for the geologic barrier *(10 CFR 60.113[a][2])* after completing the first module in the consequence analysis (Figure 3.5).

Because the compliance evaluation procedure was designed to satisfy the exacting demands of the containment section, the following text first discusses compliance with this section. Simplifications possible for the five remaining license requirements are then discussed.

Compliance with EPA Containment Requirement 40 CFR 191.13. The procedure described up to this point has generated

- Probabilities for each of the most important mutually exclusive release scenarios, n_s (scenario development and screening)
- Appropriate ranges and distributions for model parameters of important scenarios (conceptual model development)
- Predictions of the total release of each radionuclide over 10,000 yr, using parameter values sampled n_v times from their distributions (consequence analysis).

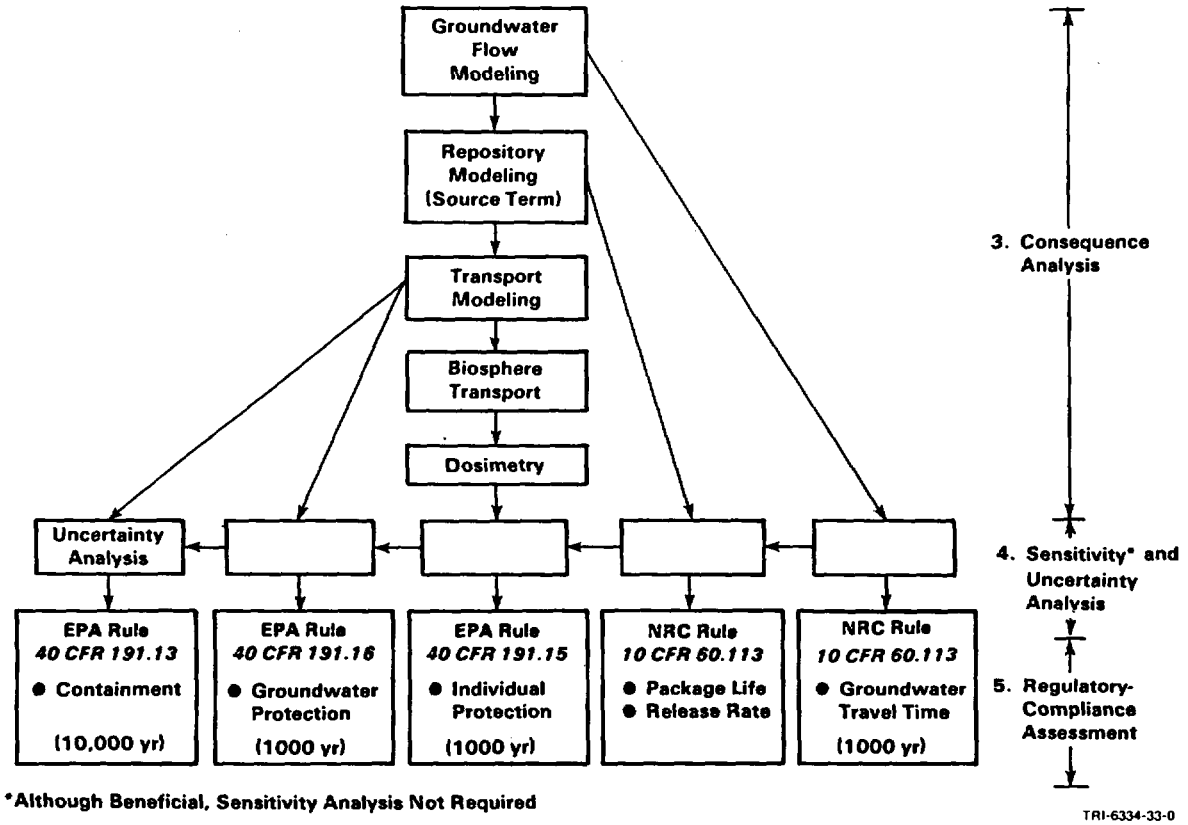

Figure 3.5 Different stages of consequence calculations used to assess compliance with requirements of the HLW regulations.

The final steps to assess regulatory compliance with the containment section ;ure 3.5) are to

- Calculate the EPA sums for radionuclide releases to the accessible environment for each of the n_s scenarios
- Generate the complementary cumulative distribution function (CCDF)
- Compare the CCDF with the release limits, L_i, of the Containment Requirements.

As described in Section 2.2, the EPA sums are calculated from

$$\hat{R}_k = \sum_{i=1}^{n_r} \frac{Q_{i_k}}{L_i} \leq 1 \text{ (or 10)}; \; k = 1,\ldots,n_v \qquad [3.8]$$

where

L_i = EPA release limit for radionuclide i

n_r = number of radionuclides

n_v = number of sample runs

Q_{i_k} = predicted cumulative release for radionuclide i for sample run k

$= \int q_{i_k}\, dt$

q_{i_k} = release at time t for radionuclide i for sample run k (see [3.1])

$\hat{R}_k$ = summed normalized releases (EPA sum) for Monte Carlo sample run k.

The CCDF describes the probability of exceeding any given value of the EPA sum, R; it is the graph of calculated EPA sums for each scenario, $\hat{R}_k$, versus the cumulative probability, $P(R_k > R)$, that $\hat{R}_k$ exceeds any given value of the EPA sum, R. The cumulative probability, $P(\hat{R}_k > R)$, is calculated as follows (Cranwell et al., 1987):

$$P(\hat{R} > R) = \sum_{j=1}^{n_s} P(\hat{R}_k > R | S_j)\, P(S_j); \qquad k = 1, \ldots, n_v \qquad [3.9]$$

where

$P(\hat{R} > R)$ = probability of predicted EPA sum, $\hat{R}$ > any given EPA sum, R

$P(\hat{R}_k > R | S_j)$ = probability of $\hat{R}_k > R$ for scenario S_j, given that the scenario occurs

$P(S_j)$ = probability of scenario S_j occurring over 10,000 yr,

where

$$\sum_{j=1}^{n_s} P(S_j) \leq 1 \; . \qquad [3.10]$$

The conditional probability, $P(\hat{R}_k > R | S_j)$, is estimated from the frequency of sample runs for scenario S_j that produce a calculated EPA sum, $\hat{R}_k$ (sample run k), greater than any given EPA sum, R (Hunter et al., 1986):

$$P(\hat{R}_k > R | S_j) \approx \frac{n_m}{n_v} \qquad [3.11]$$

where

n_m = number of sample runs for scenario S_j with $\hat{R}_k > R$

n_v = number of sample runs for scenario S_j (often the same for all scenarios).

This plotting position rule (Haan, 1977) is appropriate, since Latin hypercube sampling samples the entire distribution of a parameter with equal probability.

The predicted CCDF is generated by plotting the calculated EPA sums for sample run k, $\hat{R}_k$, versus the cumulative probability, $P(\hat{R}_k > R)$. The total number of points to plot is $n_v \bullet n_s$ (Figure 3.6). To more easily see the individual points (and as a conservative assumption), the CCDF is sometimes plotted as a step function. Hunter et al. (1986) work through a simple example problem.

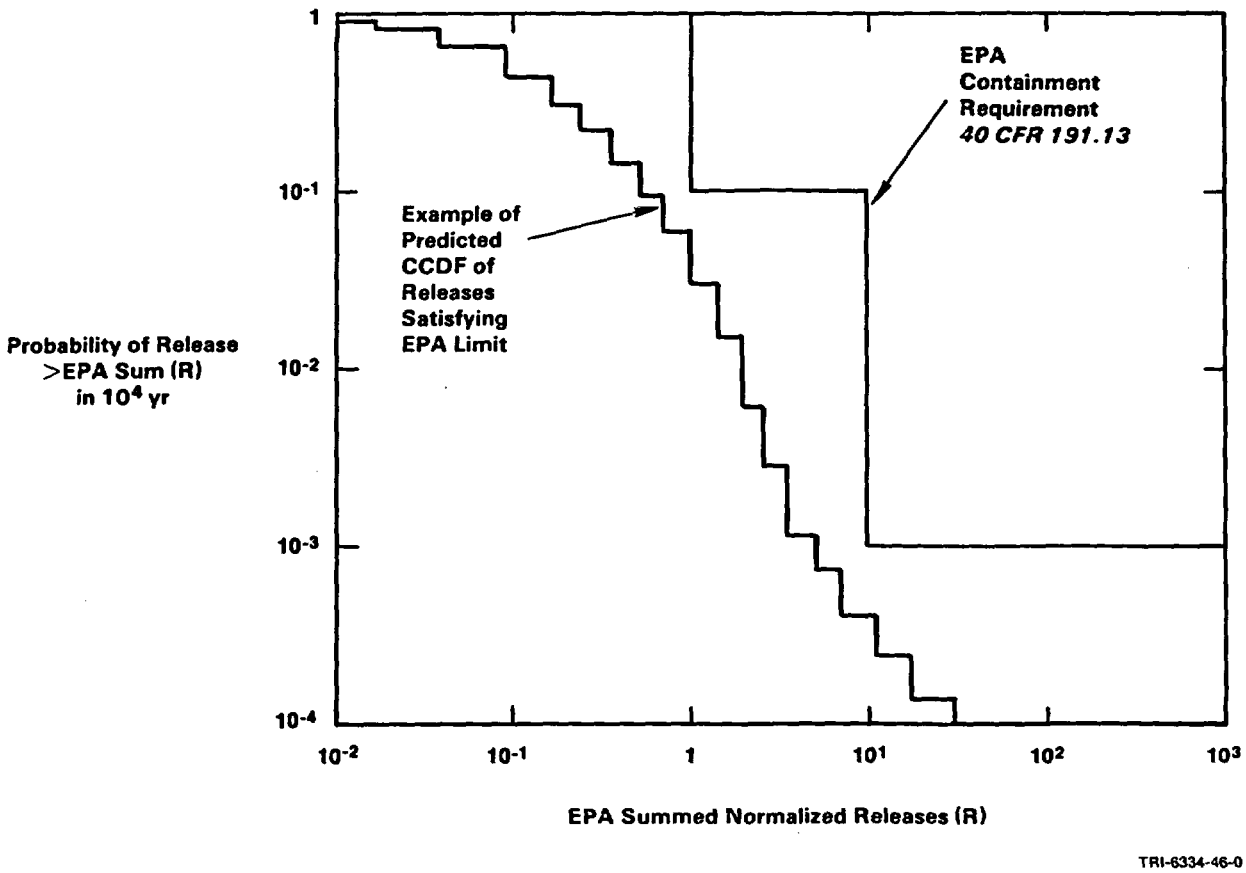

Figure 3.6 A complementary cumulative distribution function is produced for comparison with the EPA containment requirements.

Compliance with Remaining EPA Requirements. Evaluating compliance with the two remaining EPA requirements (Groundwater Protection and Individual Protection) uses the same structure, but calculations are simplified because

- Only one scenario is evaluated, the undisturbed performance (predicted behavior without human intrusion) of the disposal system
- No scenario probabilities must be estimated
- Only the behavior for the first 1000 yr must be predicted.

However, uncertainties in the parameters necessary for evaluating this scenario must still be calculated in order to calculate a distribution of results. The highest of the mean or median of the distribution of results must not exceed concentration limits for the Groundwater Protection or dose limits for the Individual Protection Requirements (*40 CFR 191,* Appendix B).

Groundwater Protection Requirement. If Class I groundwater (EPA, 1984) is within the controlled area or less than 5 km beyond, is irreplaceable, and supplies drinking water to thousands of persons (i.e., a "special" source of ground water), radionuclide concentrations within the groundwater for the first 1000 yr must be predicted.

Although predicting concentrations requires the same modules as for the containment section (hydrologic, source term, and transport modeling) (Figure 3.5), the dispersivity and release rate for the radionuclides must be fairly well known (factors deemphasized for the Containment Requirements, because the *cumulative* release is used). Consequently, more precise source-term and transport calculations may be required.

No special sources of groundwater are within 5 km of the controlled area for the WIPP (WIPP Strategy, 1988).

Individual Protection Requirement. All potential pathways to the public associated with the undisturbed performance must not result in doses greater than 25 millirems to the whole body or 75 millirems to a critical organ within the first 1000 yr. To predict potential radionuclide doses requires the addition of a biosphere (surface-water, atmosphere, and biological pathway) module in the consequence analysis task (Figure 3.5). Similar to the Groundwater Protection Requirement, the release rate and dispersivity are more influential on the uncertainty of the results than for the Containment Requirements.

Two pathways to man for the WIPP involve transport through the overlying Rustler Fm. to the Pecos River or transport to a source of groundwater (large volume, near land surface, with moderate total dissolved solids) for livestock outside the controlled area. The only credible (but still unlikely) pathway is transport to a groundwater source for livestock which permits radionuclides to enter the human food chain.

Compliance with NRC Regulations. Groundwater travel time and engineered barrier life and release rate requirements issued by the NRC *(10 CFR 60)* establish minimum performance requirements for the geologic and engineered barrier, respectively. They can be evaluated after the first two modules in the consequence analysis task (Figure 3.5). Should an NRC-regulated disposal system meet the NRC requirements, assessing compliance with the EPA Individual Protection Requirement should be straightforward for that system.

The simplifications of the calculation procedure listed when describing compliance with the Individual Protection Requirements apply to the NRC requirements as well. However, for the groundwater travel time, the fastest travel time, rather than the mean or median of the resulting distribution function when including uncertainty, must be used to assess compliance. Furthermore, for the groundwater travel time requirement, the undisturbed performance scenario excludes any beneficial or detrimental process that occurs near the repository because of the waste or facility *(10 CFR 60)*.

The TRU waste to be disposed at WIPP is specifically exempted from regulation by the NRC.

3.7 Benefits of Compliance Assessment

Benefits of the compliance assessment methodology (CAM) stem primarily from the systems analysis approach used to examine the disposal system. A few of the many ideally attainable benefits are given below.

First, because of the sensitivity/uncertainty analysis, the proper balance between intrusive and nonintrusive site characterization is easier to determine and maintain.

Second, concerns raised both within and outside the project remain in the proper perspective; without a system viewpoint, any one concern has the potential to take the project off on a tangent. For example, both the analyst and regulator can better perceive the need to devote significant resources to likely processes of moderate consequence, although still substantiating that other processes are unlikely or of low consequence.

Third, the proper balance between near-term and long-term concerns is more easily discerned (e.g., influence of room stability versus the influence of human intrusion scenarios on facility design).

Fourth, performance measures for the engineered barriers are well defined (e.g., design criteria for shaft backfill and seals).

Fifth, evaluating engineered barrier alternatives from a system perspective is possible.

Finally, the analyst and regulator better perceive that the importance of data is relative; for example, the importance of reducing uncertainty in the local hydrology is relative to what is already known about the regional hydrology. This information is important for allocating resources for data collection about: (1) regional hydrology (e.g., recharge areas, boundary conditions, model size, brine pockets, human-induced disturbances of the aquifer); (2) local hydrology (e.g., fracture versus porous media flow, local model size); (3) source term (e.g., brine influx, salt creep, initial inventory, radionuclide solubility, backfill mixture); and (4) transport/retardation properties.

4. Additional Aspects of Compliance Assessments

This chapter elaborates upon several tasks affecting data flow that were reviewed in the previous chapter. It concludes with a discussion of specific requirements of code linkage and data flow implied by the compliance assessment procedure. Chapter 5 discusses a general solution to problems discussed here that facilitated design of a data flow controller, CAMCON.

4.1 Multiple Passes in Compliance Assessment Procedure

Benefits accrue from iterating through the entire compliance assessment methodology several times (Figure 4.1). The function of early iterations (cycles) through the system is to help project managers allocate resources wisely for data collection and modeling development. Although the final compliance assessment may need detailed data and precise models, the first pass is only preliminary, making use of sparse data and simple conservative models. However, scenario development must be thorough on the first pass because much insight about the disposal system is gained at this step.

Subsequent passes through the compliance assessment system update the screened list of scenarios, while making use of more detailed models and the insight gained from earlier sensitivity analysis (Figure 4.1). Here the system-wide sensitivity analysis provides insight into the influence of the uncertainty of a process on assessing compliance, whereas the sensitivity analysis used during design modeling iterations provides insight into the individual process (both types of sensitivity analysis were mentioned in Chapter 3).

Iterations concerning site characterization and facility design can occur more frequently than iterations through the entire system. For the WIPP, two or three iterations through the system are planned, whereas numerous process-modeling studies have already examined important processes and experiments begun for validating a few model components.

Although Figure 4.1 shows the iterations necessary for compliance assessments, a network diagram is needed to show the interaction necessary between the site characterization, facility design, and waste characterization and the compliance assessment. Figure 4.2, a simplified hypothetical network diagram for a compliance assessment, shows some of this interaction but omits the time scale--an important constraint. Furthermore, experiments for site characterization and consequence assessments are lumped together, which neglects the difficult task of allocating resources between these two types of experiments.

Early compliance assessments provide feedback for experiments performed for site characterization and facility design. Because of the size of the experiments, the feedback may affect the completion time and/or cost. Furthermore, if a major redirection is suggested by a preliminary compliance assessment, factors other than the scientific input provided by the assessment (e.g., cost, public perception, and politics) will have to enter into any decision to redirect experiments--a time-consuming process.

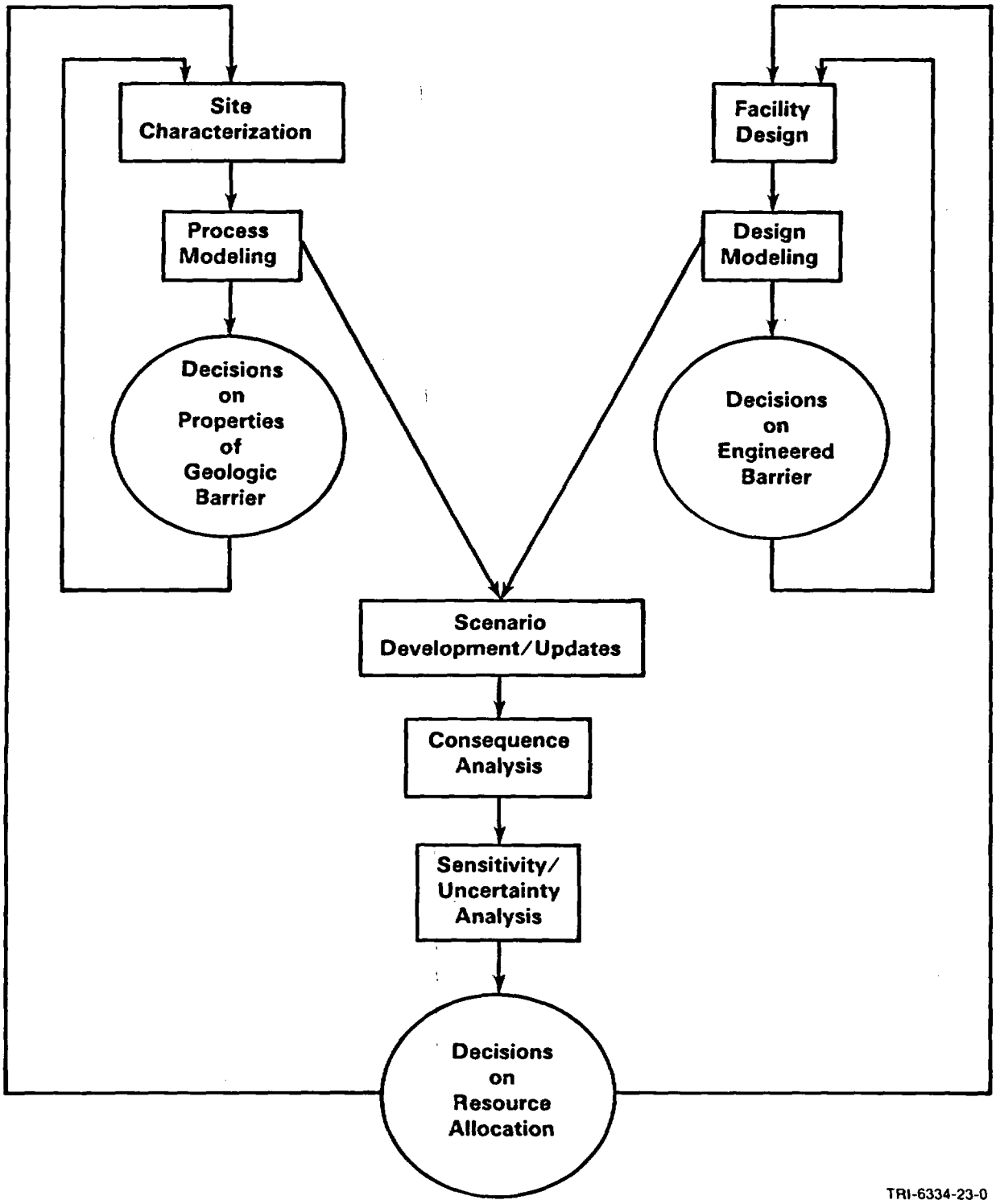

Figure 4.1 Better resource allocation occurs when iterating through the compliance assessment system in addition to iterating through the site characterization and facility design process.

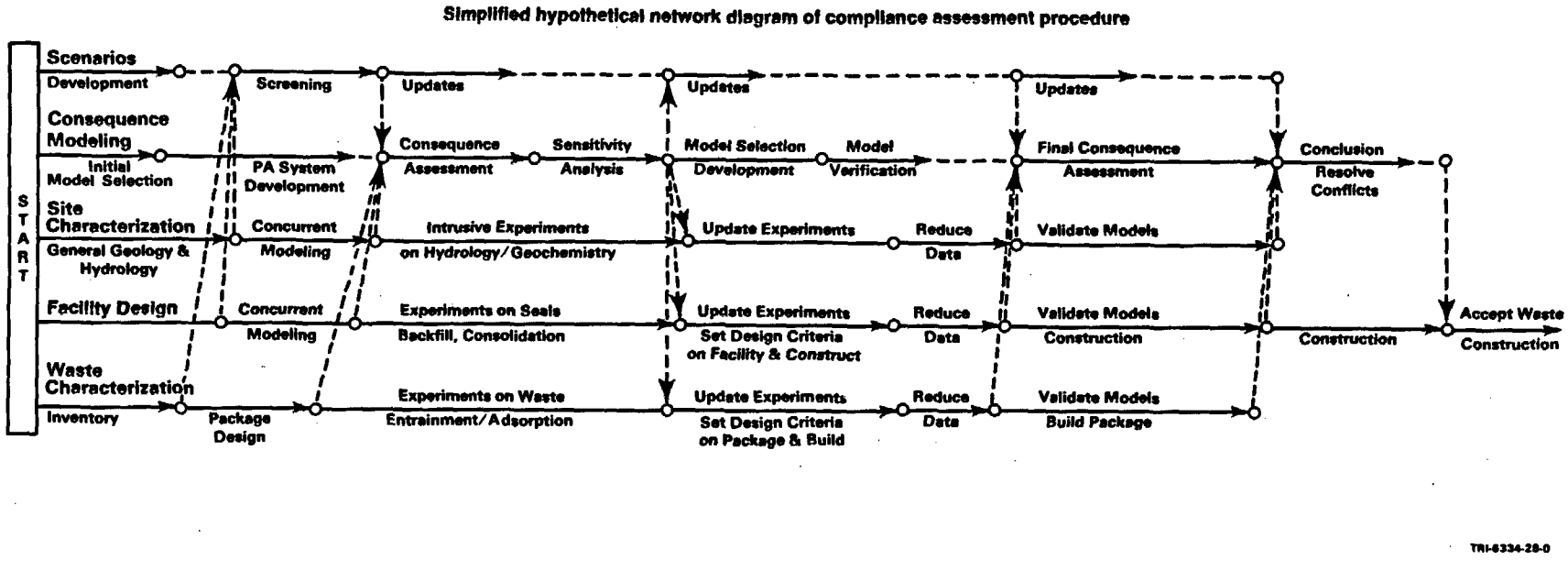

Figure 4.2 Simplified hypothetical network diagram showing interaction between compliance assessment methodology (scenario development and consequence modeling) and disposal system characterization (facility design and site and waste characterization).

4.2 Monte Carlo Sampling

As previously described, the SNLA CAM propagates uncertainty and analyzes parameter sensitivity using Monte Carlo sampling, specifically, Latin hypercube sampling (LHS) with restricted pairing (Iman and Conover, 1980). The ideal approach to LHS sampling is to generate the sample vectors of varying parameters across all scenarios at the same time. Then each scenario simulation uses identical sampled parameters (e.g., each scenario uses a large hydraulic conductivity for the Culebra Dolomite member of the Rustler Fm. at the same time). Parameters unneeded in any one scenario are ignored. This sampling scheme has two advantages:

- Variations between scenarios can be attributed solely to the scenario, because no differences exist between the generated sample vectors
- Sensitivity analysis to determine important variables across several scenarios can be performed.

The importance of these advantages varies. For instance, the importance of identifying the cause for differences in releases between scenarios decreases as the number of common physical characteristics decreases. Likewise, the importance of performing sensitivity analysis across all scenarios decreases as the number of common parameters decreases.

One major disadvantage with simultaneous sampling for all scenarios occurs because of management logistics. When sampling is done all at once, all scenarios must be well understood and the consequence codes completely assembled to select the parameters to vary--a difficult task when many scenarios must be examined that involve different types of codes.

Consequently, the planned approach for Monte Carlo sampling for the WIPP compliance assessment is as follows:

- For all preliminary assessments, sample separately for parameters in each scenario
- For final assessment, sample across all scenarios simultaneously.

The main point to understand here is that flexibility in the order of performing calculations must be maintained throughout the consequence analysis.

4.3 Model Subdomains in Consequence Assessments

A three-dimensional model with the necessary detail to analyze hydrologic processes (or transport) both far from and near to the repository for every scenario would take too long to build, modify, and solve--points intuitively obvious. Hence, models are scaled to a specific scenario to make the analysis tractable. However, disposal system analysis entails an additional complication: using different model scales or subdomains that must pass pertinent results to each other. The code modules associated with the different subdomains are in addition to those required for evaluating different processes such as radionuclide transport.

Although not a common technique, other large computational problems such as atmospheric or oceanic forecasting require similar modeling subdomains that communicate with larger-scaled models. For example, for oceanic forecasting, an ocean basin model was used to evaluate fluid motion and energy transport throughout the ocean basin, while local models were used to evaluate turbulence in small areas of concern (Marietta and Simmons, 1988; Dietrich et al., 1987; Marietta and Robinson, 1986).

For disposal systems, three scales are frequently used (Figure 4.3):

- Regional
- Local
- Repository.

Regional Scale Model. The primary function of the regional scale model is to establish groundwater flow patterns in a large region bounding the controlled area of the repository. The regional model establishes the major flow paths bounding the repository. The flow conditions (e.g., heads, fluxes, or brine densities) are then used to establish boundary conditions for the next scale model, the local model.

The regional model domain must be large enough to accommodate the important aspects of the scenario being studied (e.g., climatic changes affecting recharge or stock water wells), yet small enough to remain tractable. In addition, the grid spacing must be fine at the boundary of the local model to ensure accurate transfer of information. Furthermore, the boundary conditions (e.g., limits of aquifer, groundwater divides, head and flux boundaries such as rivers and lakes, or possibly well data) must be known fairly well to reduce uncertainties in the computational model. For transient analysis, the necessary maximum size is also controlled by how fast transient boundary condition effects produced at the regional boundaries can reach the site and affect local flow and transport.

Local Scale Model. The function of the local scale model is to more precisely predict the flow field within the controlled area for transport calculations. The local scale model is completely embedded within the regional scale model. The modeled features such as stratigraphic layering are more refined than in the regional model to more precisely predict the flow field. The head or possibly other conditions such as flux or brine density at the boundary of the local model are derived from the regional model.

The local scale model encompasses at least the controlled area of the disposal system, but areas outside the controlled area necessary for modeling physical processes potentially disrupting the hydrologic system may also be included. Encompassing these areas within the local model reduces (but does not always eliminate) the need to interpolate back into the coarsely gridded regional model.

Repository Scale Model. The primary function of the repository scale model is to calculate migration of radionuclides (or other hazardous waste) from the consolidated waste-disposal rooms through the seals, drifts, and shafts--assuming the fluid fields (i.e., antecedent heads, fluxes, and brine densities) calculated by the local model (or other repository scale model). The time versus radionuclide concentration curves are then used as a source term for evaluating transport with the local scale model.

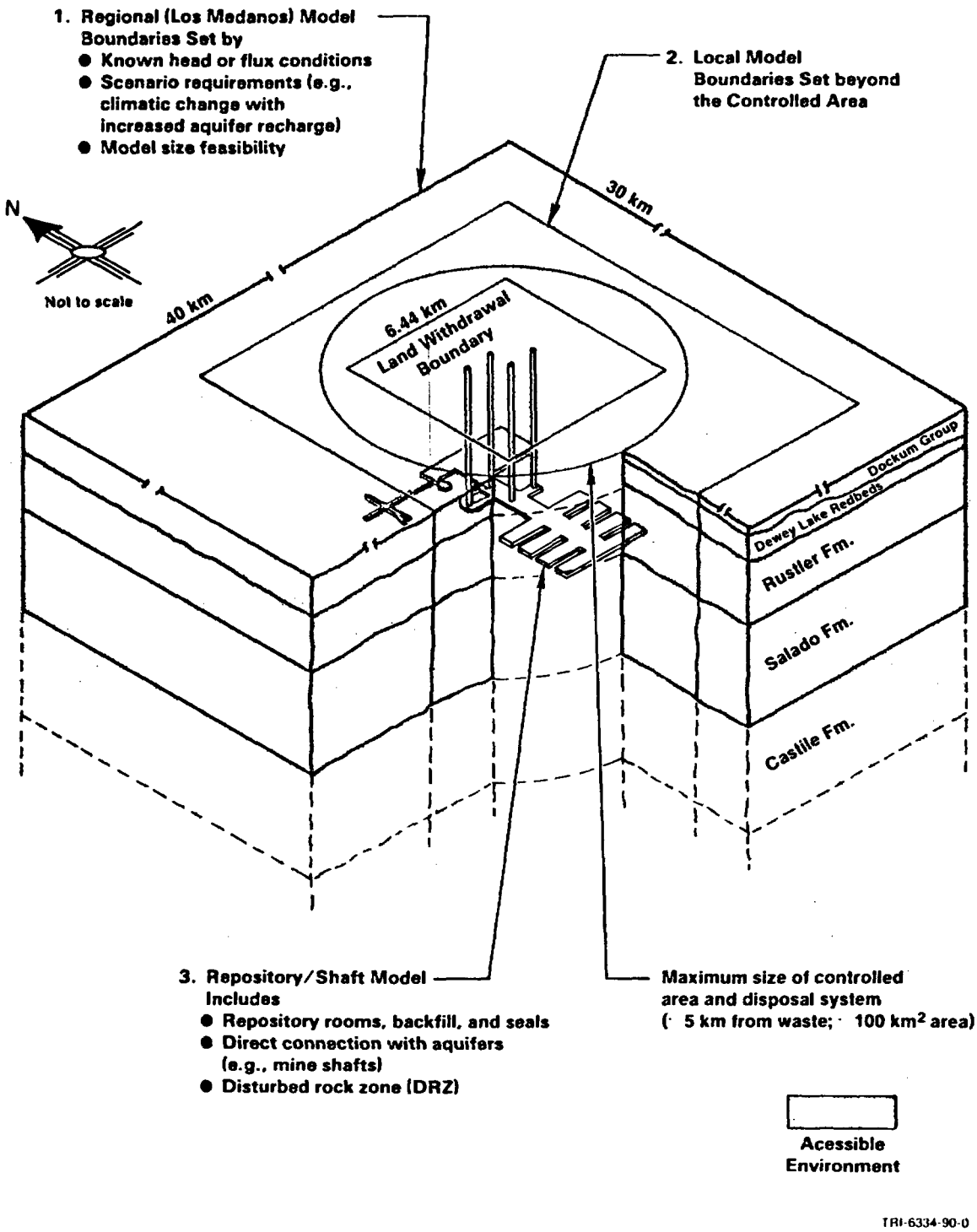

Figure 4.3 Three model scales are typically used in compliance assessment (after Bertram-Howery and Hunter, eds., 1989).

The complexity of the physical processes affecting the repository requires that initial source-term calculations involve several codes modeling various coupled processes carefully linked together (e.g., creep consolidation of the rooms coupled with resaturation)--in other words, a microcosm of the overall compliance assessment.

For the WIPP project, the complexity of the repository component rivals that of the overall system; consequently, much work is required to explore the importance of various phenomena and to develop a module appropriate for use in the overall compliance assessment. The relative importance of four phenomena must be determined (Figure 4.4):

- Mechanical, including
  - Creep closure and consolidation of disposal rooms
  - Reconsolidation behavior of backfill and seals
  - Healing of the disturbed rock zone (DRZ)
  - Deformation of waste drums
- Hydrologic, specifically, resaturating brine flow into rooms
- "Chemical," including
  - Amounts of radioactive, organic, and inorganic components
  - Adsorption of radionuclides in backfill and host salt
  - Dissolution and entrainment of radionuclides
  - Generation of gases from corrosion and radiological and biological decomposition
- Transport, including
  - Diffusion
  - Porous or fractured media flow.

Furthermore, four major model components incorporating various aspects of the above four phenomena* are anticipated for the WIPP (Figure 4.4):

- Room model
- Panel seal model
- Drift backfill model
- Shaft backfill and seal model.

These model components must be linked together to look at the repository as a system. For example, an analysis of one room must be expanded or scaled to represent all rooms. This system-level viewpoint is, in turn, important for developing a fast-running surrogate model for use in the overall compliance assessment. Furthermore, the system-level viewpoint is important for establishing clear performance measures for the repository design. For example, the relative importance of panel and shaft seals must be established from a system level through a sensitivity analysis.

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*Evaluating the importance of the four phenomena is similar to accident analysis for nuclear power plants.

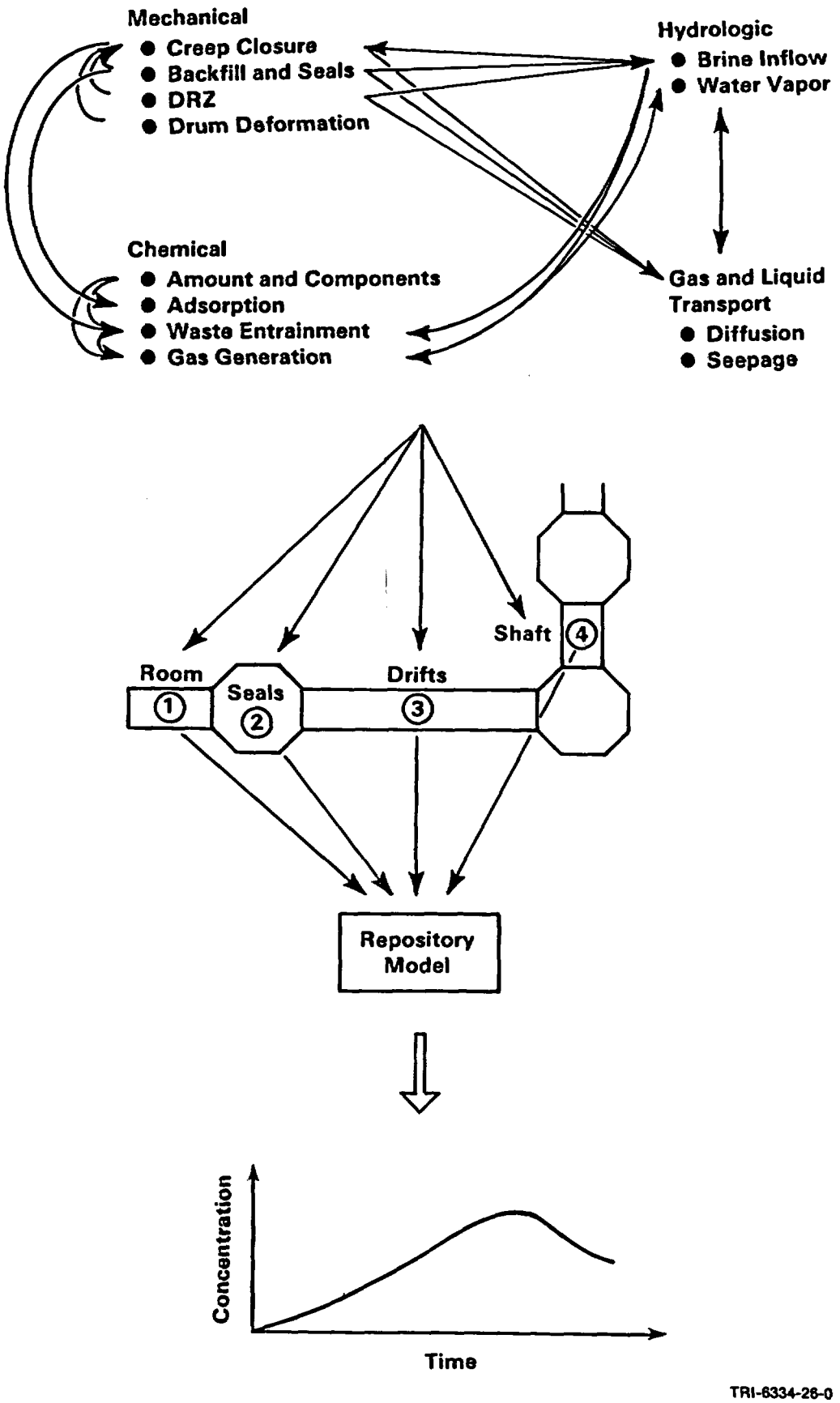


Figure 4.4 Repository modeling component must be assembled from four submodels.

Ideally, the same computer controller developed for the overall compliance assessment can be used to explore the repository module with only minor modifications.

Setting Boundary Conditions. Embedding models can reduce unnecessary model complexity (operations per grid point per time step) and thereby model run times. However, when embedding models, an important process which affects the flow of data is setting boundary conditions. The development of interpolation programs is not trivial. Several questions must be answered:

- How will changes in vertical resolution of stratigraphy between the regional and local model be handled?
- How will time scales between the local and regional models be separated to permit different time steps, thereby increasing computational efficiency?
- How many surrounding grid points will be included in spatial interpolations?

To elaborate on the first question, when interpolating between the regional and local models, it is possible that the stratigraphic layers will be grouped differently in the regional and local scale models (e.g., greater vertical resolution in the local model), thus using different material parameters. However, for Monte Carlo sampling, the properties for materials in the two models must be consistent (very highly correlated) to properly interpolate between the two models. The easiest solution is to sample the original stratigraphy, and then combine the material properties appropriately for the stratigraphy for the model under consideration (using the combined properties for sensitivity analysis).

Interpolating from Coarse to Fine Grids. The process of embedding meshes as previously described involves interpolating from a coarse grid to a fine grid--just the opposite of what is mathematically convenient. Simple or complex schemes can be devised to accomplish this task. However, both the simple and complex interpolation schemes can cause discontinuities in the fields--the simple by ignoring too much detail, and the complex by fabricating more detail than is warranted from the information contained in the coarse mesh. The correctness of the interpolation is best surmised by plotting the behavior of fields at the interface.

Interpolating from Fine to Coarse Grids. Although the predominant direction for interpolating is from the coarse to the fine meshes, two cases require information to flow from fine to coarse meshes:

- Transporting radionuclides from the local into the regional mesh or from one subdomain into another subdomain
- Iterating between local and regional hydrologic models.

Concerning the first case, ideally the local mesh encompasses enough area to preclude the need to track radionuclides from a local into a regional model. However, if the local mesh is divided into computational subdomains (for cost-effective computing), this step might be required.

The second case, adjusting boundary conditions at the interface between the local and regional meshes by iteration, is a possibility for the WIPP, because extensive hydrologic testing was done to establish a calibrated local scale model (Haug et al., 1987). Analysts wish to explore the possibility of propagating

the information contained in this calibrated model into the regional model. However, the calibrated model represents one of several possible solutions not unique to the hydrologic test conditions. Hence, rather than fix internal boundary conditions on the regional model at the interface between the two models (implying that the local model boundary conditions are correct), WIPP analysts must iterate between the local and regional model solutions at the interface (Figure 4.5). Experience with embedding ocean models suggests that this will only involve two or three iterations (Marietta and Robinson, 1986). Understandably, the local model may need to be recalibrated after adjusting the boundary conditions on the local model.

4.4 Requirements for CAMCON: Controller for Compliance Calculations

Based on the compliance assessment procedure described in this and the previous chapter, an executive program to aid in consequence calculations is needed to meet several requirements. Generally, the requirements can be grouped into two categories: built-in flexibility and built-in quality assurance (QA) features. Specifically, an executive program must

- Accurately link several distinct model components with little analyst intervention (QA)
- Trace the calculations so that they can be repeated (QA), in addition to software QA features on individual modules
- Propagate uncertainty by Monte Carlo analysis, uniquely identifying calculations to avoid misinterpretation (QA and flexibility)
- Permit an analyst to examine a large number of intermediate and final results (QA and flexibility)
- Allow interpolation between modeling scales (flexibility)
- Permit iteration between computer modules (flexibility)
- Aid in exploring phenomena of computer modules (e.g., of the repository model) (flexibility)
- Be flexible in switching computer modules to aid in scenario screening, model/model comparisons, sensitivity analysis, and fine-tuning of the system for final compliance assessment calculations.

In other words, the variety of scenarios analyzed, the varying complexity of models used, and the need to switch codes when cycling through the procedure are characteristic of compliance assessments that require a flexible and versatile implementation. Furthermore, the number of repetitive computer runs, the need to properly identify runs, and the need to recreate runs are characteristics that require adequate quality assurance implementation.

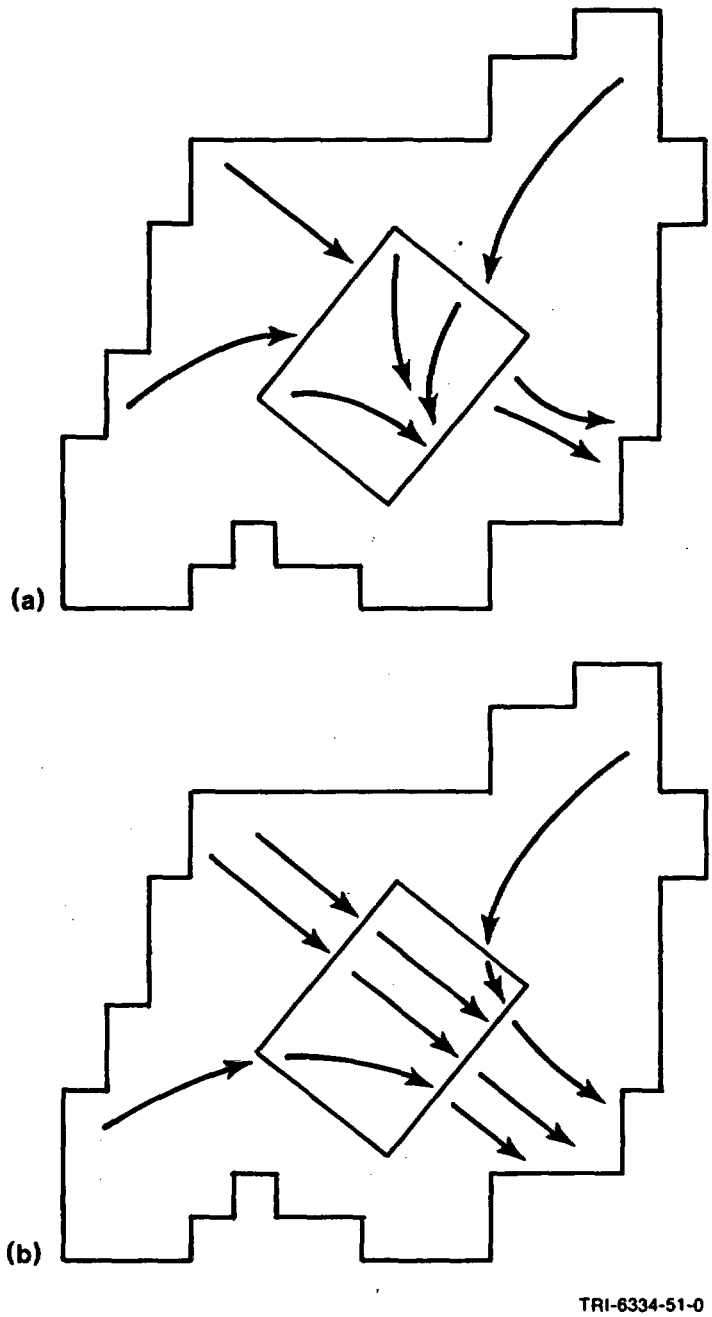


Figure 4.5 The WIPP will explore propagating information from a calibrated local model into the regional model by iterating boundary conditions at the interface between the local and regional hydrologic models: a) disagreement between calibrated local and regional models, b) agreement after iteration between recalibrated local and regional models.

Furthermore, several general modeling difficulties affect the storage of data used by CAMCON. These include

- Spatial variability of parameters in a geologic medium
- Transient behavior
- Varying the order of events in a scenario
- Time varying parameters.

Aspects of all four modeling difficulties may be present at the WIPP.

For example, at the WIPP the overall variability of the transmissivity of one layer, the Culebra Dolomite member of the Rustler Fm., varies about 5 orders of magnitude across the 30-by-40-km area represented by the regional model (Brinster, 1989). Yet, this variation exhibits a trend with less than a two order-of-magnitude variation. Concerning transient behavior, geochemical data suggest that the Culebra member is still responding to a change in recharge after the last pluvial period, suggesting that the flow field around the site is still transient (Lappin, 1988; Lambert, 1988).

Consequently, some provision was made in the computational data base to aid calculations exploring the first two difficulties. First, although there is no straightforward way of inputing property trends in a "random" manner, the implication for the design of the computational data base was clear. Variations of a hydrologic property such as transmissivity within one material require that properties be stored on an element basis instead of on a material basis (using zones of materials would be another approach). Second, exploring the importance of transients to the radionuclides migrating from the site requires a data base capable of storing transient results. The third and fourth modeling difficulties will be handled outside the computational data base.

The basic approach proposed is to modularize the tasks both conceptually and practically so that code modules are interchangeable, making the system design open-ended. Chapter 5 describes the computational data base used by CAMCON that facilitates this flexibility while maintaining computational quality.

5. Assuring Accurate Data Transfer

The quality of the compliance evaluation must be high. The best strategy for meeting this goal is to build in quality. In addition, the tools given the analyst should be capable of providing the quality of work expected. This chapter describes in general terms the quality features built into data transfer. Chapter 6 describes many of these features in detail.

The quality of the compliance evaluation depends on the quality of the data in the data bases. For this report, these data bases have been grouped into three general categories:

- Primary
- Secondary
- Computational.

By categorizing the data, an analyst is better able to locate and control uncertainties in the data (principally in the primary data base), conceptual models (principally in the secondary data base), and computational models (principally the models in the compliance assessment system). All the uncertainties combine to produce the uncertainty in the results (see Figure 2.3).

5.1 Primary Data Bases

Requirements. Primary data bases contain the measured field and laboratory data gathered during the disposal system and regional characterization step of the compliance evaluation described in Chapter 2 and shown in Figure 5.1. Several requirements exist for the primary data base:

- The quality of the data must be very high
- The data base must contain all data necessary for the compliance assessment
- The data in a primary data base should have as little subjective interpretation as possible
- The structure must be flexible to accommodate various organizations of data and unforeseen data types
- The structure must be easily understood and accessible.

The justification for these five requirements follows.

First, the quality assurance procedures for the primary data base must be very high, because the analysis can be no better than these data. Data gaps and numerical modeling assumptions cannot increase the accuracy of the analysis. Because of the length of time required to characterize, design, and assess the feasibility of a disposal system, staff turnover is a factor. Thus, the data base must function as a corporate memory.

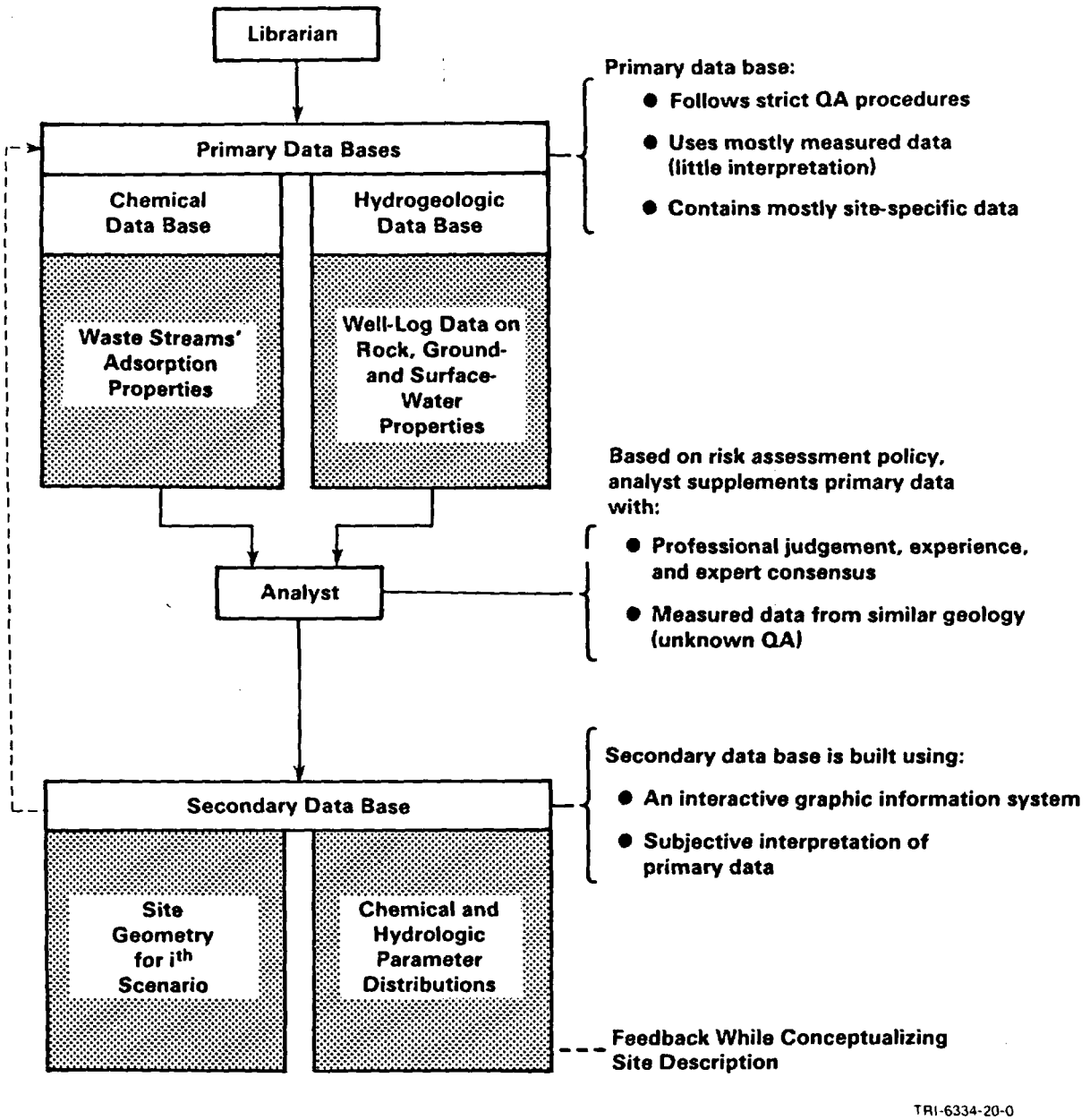


Figure 5.1 Analyst interprets data in primary data base to develop secondary data base.

Second, the purpose of the primary data base is to compile data necessary for performing the diverse analyses of the compliance assessment. Although the purpose is self-evident, reaching a consensus among the participants (representing such diverse disciplines as geology, hydrology, geochemistry, mining engineering, and mechanical engineering) as to which constitutes the necessary set of data is not a straightforward process.

Third, because the interpretation of test data can vary as the conceptual model of the disposal system changes (e.g., most parameters used in hydrologic studies are not physical properties, but model

parameters that depend upon the "viewpoint" of the model), ideally only test results are stored in the primary data base. However, storing uninterpreted data can only be approached as a goal, not a reality, because of the large amount of data involved. Reaching a consensus on the degree of interpretation permitted is not straightforward. Consequently, sources for original test data must be included.

The fourth requirement is that the structure be flexible, to accommodate unforeseen data needs and organization. A relational data base is suggested, but even within relational data bases, the contents of various tables can vary. Practical experience suggests that tables containing one parameter (e.g., hydraulic conductivity) or a group of closely related parameters (e.g., Young's modulus and Poisson's ratio) are best (Rautman, 1988).

Finally, the data base serves as a central repository of data for diverse disciplines and must be stored in a form readily understood by the various analysts. The data base must be readily accessible to the analysts, since varying conceptual models (embodied in the secondary data base) will be constructed from these data for the various scenarios as understanding about the disposal system changes. Furthermore, oversight groups unfamiliar with the data base structure will require access to the data.

Suggested Format. Based on practical experience (Rautman, 1988), the four proposed components of each relational table in the primary data base are

- Parameter location
- The parameter and units of measure
- Test conditions and supporting information
- References and miscellaneous.

The first section of the table locates the parameter spatially. Because a drill hole name and depth are easily understood by most users (and can possibly be deciphered even when a typographical error occurs), their use is proposed for locating the parameter. However, some data, such as climatic and biologic data, are not associated with a drill hole and would require a slightly different location scheme. A sample number can also be used to identify a particular specimen.

The second section contains the single measured parameter value and the units of measure. Retaining the original units of measure eliminates some QA concerns.

The third table section tabulates information on the parameter measurement (e.g., an ID for the measurement technique or specific conditions such as sample size and saturation). Storing test conditions allows an analyst to carefully discriminate between parameter values.

The final section of the table stores QA information such as source document, entry date, and QA level or alternately an index code for locating more detailed information in a record center. Any comments on data can be included here, if necessary.

In summary, an example form for a file in the primary data base would be: Drill hole name; Depth; Parameter value; Units; Test ID; Source document.

5.2 Secondary Data Bases

Development of a Secondary Data Base. The analyst evaluates and interprets the data in the primary data base to arrive at a conceptual model of the disposal system for each scenario; the secondary data base is composed of bits of information that make up the conceptual model. In other words, the secondary data base embodies the conceptual model.

The levels of interpretation can vary from objective interpolation of data (techniques easily reproduced by others) to subjective extrapolation of data (not easily reproduced by others unless well documented). Data from literature, professional judgement, experience, or consensus are used to bridge any remaining gaps in knowledge, so that a complete conceptual model is available (Figure 5.1).

Developing a conceptual model is a lengthy, arduous task. Furthermore, it is a poorly defined process subject to initial unknowns about the system. Developing a conceptual model and, thus the secondary data base, continues until the final compliance evaluation takes place.

Separate Files May Exist for Each Conceptual Model. Conceivably, each scenario may require a distinct secondary data base, because different parameters and modeling subdomains of the disposal system are needed to describe the different processes involved. For example, an analysis of groundwater dissolution will require a different subdomain of the disposal system, will group stratigraphic layers differently, and will require different properties for these layers than an analysis of salt-creep closure of the repository. Consequently, conceptual models will differ, and several secondary data bases are anticipated for the preliminary compliance assessments described in Chapter 4.

The ideal approach to Monte Carlo sampling is to determine the number of parameters to be sampled across all scenarios and sample only once. Parameters unneeded in any one scenario are simply ignored. Hence, for the final assessment the secondary data base will be divided into two separate files. One file will contain the parameter distributions needed in all the scenarios, and the other file will contain the geometric description of the disposal systems needed for analyzing any particular scenario; many different geometric files will still exist.

General Features of a Secondary Data Base. Only two general requirements exist. The secondary data base must

- Be accessible to both the analyst and executive computer package controlling the compliance analysis
- Accommodate two distinct types of data--conceptual model stratigraphy and parameter distributions (Figure 5.1).

To accommodate these two requirements, the WIPP secondary data base

- Uses an ASCII file format
- Is readable with list-directed FORTRAN read statements
- Uses two separate file formats to store model stratigraphy and parameter distributions.

Data are stored in ASCII format, making data entry and modification easier. The analyst can access the file either directly through a computer system or through a data base editor. Furthermore, the executive package, CAMCON, can easily access the data.

Because the data will constantly change, two separate file formats are also used to make editing easier and reduce the chance for random errors corrupting other sections of the data base. More importantly, because the parameter distributions will likely remain the same for many scenarios, this block of data can be separated from the model stratigraphy.

Appendix B describes in detail the file format used for storing parameter data for the WIPP. However, the components of each line of data are fairly simple:

- Parameter and material IDs
- Distribution information (mean, low, high, type of distribution)
- QA information (data source, date of entry, analyst).

Ideally, an interactive graphic information system (IGIS) would be used to help develop the conceptual model stratigraphy from the primary data base. If this were the case, model stratigraphy storage would be dictated by the IGIS system, so a file structure is not defined here. However, for the WIPP a point-grid system similar to the computational data base, described next, is used.

5.3 Computational Data Base

This chapter, the next chapter, and Appendix A describe in detail the last category of data bases, the computational data base (more succinctly named CAMDAT, Compliance Assessment Methodology DATa base). The reasons for using a computational data base follow.

Serial Linkage of Codes. Because of the interdisciplinary nature of compliance assessments, rarely has a complete series of codes been developed to easily transfer data. Hence, when linking codes in series, output from the first code must be translated into the proper input format for the next code. This two-step process, reading the output of the first code and writing the input for the second code, can easily be performed by one translator (or coupler) program. This serial connection is often the most natural quick choice (Figure 5.2). However, there is another option.

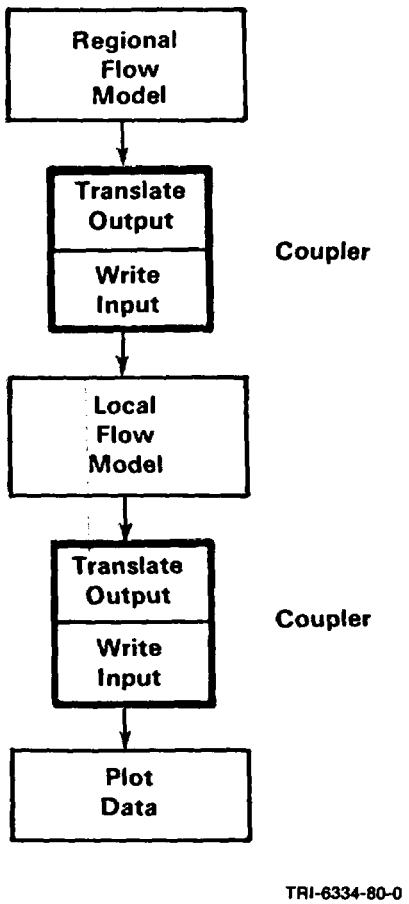


Figure 5.2 Serial coupling of codes is standard but not always ideal.

Neutral File Linkage of Codes. The two functions, translating output and translating input, can be separated and the pertinent data stored in a computational data base (a "neutral file" format) (Figure 5.3). This "zig-zag" connection (data flow approach) offers five advantages:

- Only one plotting code is needed to display results
- Codes and the order of applying codes are easily changed
- Iterating between results of codes is more feasible
- Design of a controller to automate compliance analysis is facilitated
- Assuring quality is easier.

One Plotting Code. Only one plotting code, which reads the computational data base, is needed to display any intermediate or final results from the many codes linked together. This allows more resources to be devoted to code development, and a more useful plotting package results. Furthermore, this plotting package has only to be learned once, whether plotting intermediate or final results, which increases the analyst's efficiency.

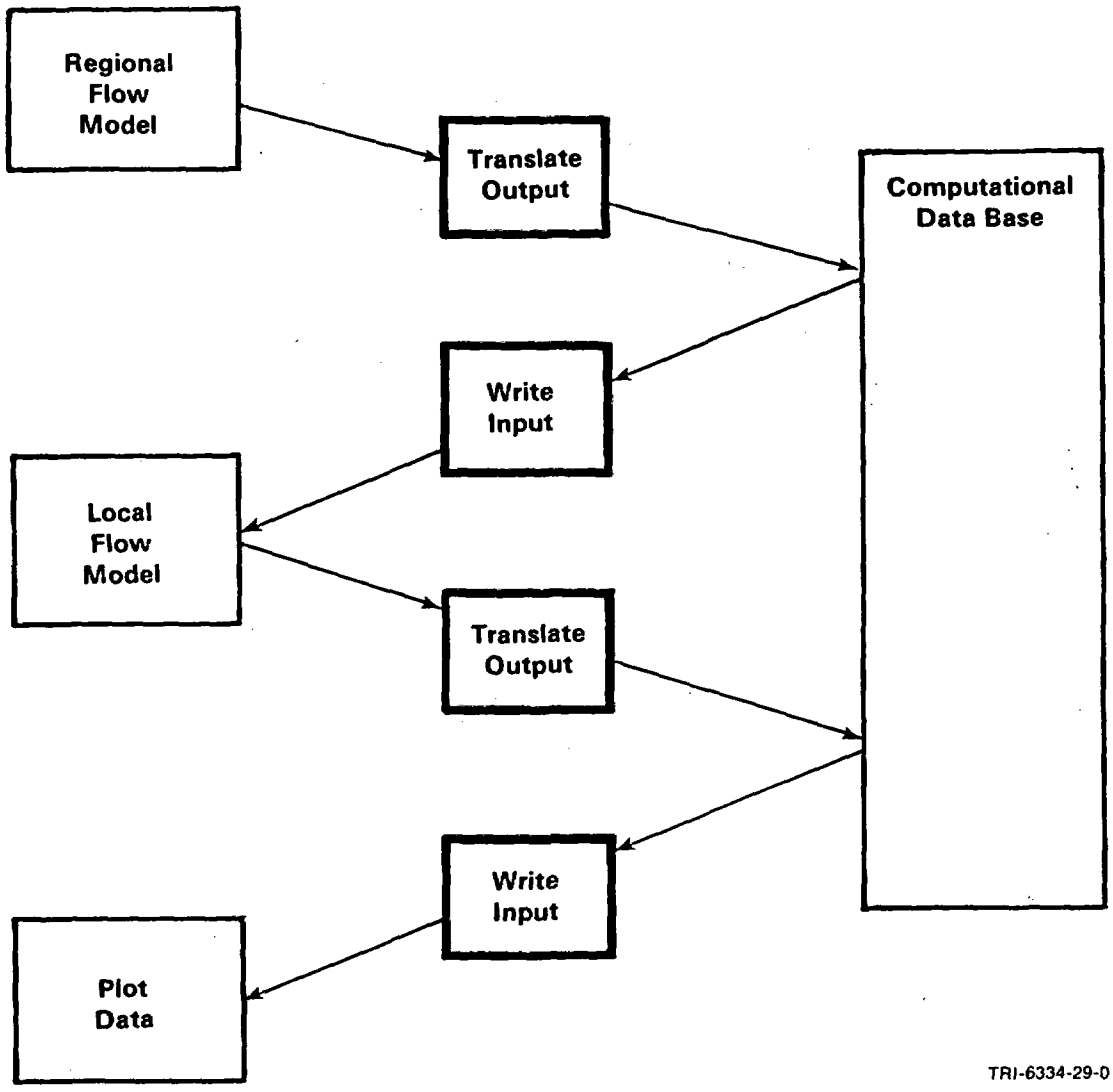


Figure 5.3 Coupling through a computational data base ("neutral file") creates a modular structure.

Codes Easily Changed. Using a computational data base permits codes to be easily replaced because when swapping codes, completely new translators with well-defined goals can be written; a programmer need not patch up previously existing software. To elaborate, a programmer saves time by not needing to first understand a previously written translator to replace an old code with a new one; he merely writes new translators between the computational data base and new code.

The functional details of the translators will vary for each computational module of the compliance assessment. Ideally, a code module would be written so that it can read and write directly to the computational data base, entirely avoiding the need for a translator.

However, for the WIPP, most major modules predate the computational data base. To avoid seriously complicating quality assurance by modifying coding, a translator is written that created the ASCII input

control cards by reading the data base and a supplemental program control file. Another translator is written to convert the ASCII output of the program module into the data base format.

A distinct disadvantage of this approach is the limited ability to build a robust input translator to make use of all features of a general purpose code, especially if the code uses an archaic method of controlling features and lacks default values. However, only when the module is well understood should a quality-assured code be modified (and quality-assured again) to read the data base directly.

When examining the flow of data as described, it must be understood that the algorithm for assessing compliance of a disposal system has been made not only conceptually modular (as described in Chapter 3), but modular in a practical sense also, because the flexibility to replace codes is built in. Furthermore, if it makes sense to do so, the order of applying codes can easily be changed.

Code Iteration More Feasible. Iterating between the results of two codes is more feasible, since the codes talk to each other through a data base. This greatly increases the flexibility of the compliance evaluation algorithm.

Controller Design Facilitated. Design of an executive package to automate the analysis is facilitated when all information resides in one data base. By using CAMDAT to carefully control data flow, building an executive package to couple the codes together and run them is straightforward. For WIPP compliance assessment, this driver is called CAMCON (Rechard, 1989). Because CAMCON was written at the computer system level, much of the coding is specific to the SNLA computer environment (VAX/VMS and CRAY). However, the concepts are transferable.

Admittedly, even poorly thought out data flow can be made to run as conveniently as a neutral file interface, but the effort is much greater. Furthermore, difficulty in understanding, maintaining, revising, or moving the methodology to another computer system may be too costly to do at all.

The purpose of CAMCON is to allow an analyst to properly build and execute portions or all of a compliance assessment for any specific scenario. Assessing any one scenario may or may not be rapid with CAMCON, however, because the difficulty and time required are dependent on the complexity and data requirements of the models (either analytic or numerical) chosen as components in the compliance evaluation. In a sense, the level of complexity of the models chosen determines how friendly CAMCON is to use. Hence, CAMCON can only approach the convenience of other compliance assessment packages such as SYVAC (Sherman et al., 1986). Moreover, the use of individual codes in CAMCON requires that CAMCON be written at a computer system level.

However, these problems are not always a shortcoming; the modular aspects of CAMCON and the WIPP compliance assessment methods make it easy for an analyst to select the proper mathematical rigor and choose from numerous existing codes when representing the conceptual model of the site. The need for this versatility at the WIPP prompted the development of CAMCON.

Assuring Quality Easier. Assuring the repeatability and quality of the analysis is made easier when all data pass through one data base, because information about all modifications of the data is recorded in a consistent format and stored in one location.

In summary, the advantages of a computational data base, CAMDAT, center around efficient use of software development resources, analyst efficiency, management of code development when codes are replaced, and quality assurance of the analysis.

General Features of Computational Data Base. The precise structure of the computational data base can vary with applications, but for evaluating compliance of a geologic repository, two main features are required:

- Ability to keep track of codes which have written to the data base to provide a trail for QA
- Versatility to handle data from different types of codes (e.g., finite-difference fluid flow and finite-element structural analysis codes).

The first feature ensures that any program writing to the file also writes a record in the file identifying itself. These records can then be printed out when plotting results. This quality assurance aspect is especially important when making numerous Monte Carlo simulations, where results may vary only slightly and the analysts can easily misidentify and thus misinterpret a simulation.

The second feature ensures a fairly versatile file format that has been extensively tested. Because of the manner in which codes are typically linked in a compliance evaluation, the order and types of information required are (Figure 5.4):

- Geometry data for finite-element (FE) or finite-difference (FD) meshes
- Geologic and hydrologic properties (material properties)
- Model boundary conditions
- QA information
- Results from fluid flow modules (velocities and heads)
- Initial concentrations from source-term modules
- Descriptions of particle pathways from transport modules and nuclide concentrations.

As mentioned earlier, a complicating factor is that up to three different model scales are used: regional, repository, and local. Each model stores similar results that must be accessible to the other codes. This problem is handled by using three separate files, all with the same file format, but with a file header indicating the model scale in the computational data base.

The file format chosen for CAMDAT was based on GENESIS (Taylor et al., 1986) and EXODUS (Mills-Curran et al., 1988), developed by SNLA's Engineering Analysis Department for the finite element computer codes. This file format was chosen because it

- Has demonstrated versatility in handling fluid and solid mechanics codes, multiple element types, and various boundary conditions
- Has a sequential file format to keep the file structure simple and easy to use for programmers
- Stores data as unformatted binary for space efficiency
- Has a file structure that defines the length of all records before the record is read, implying that the reading program can dynamically allocate memory for all arrays
- Is actively maintained by SNLA's Engineering Analysis Department with powerful data manipulation and plotting codes already available (e.g., Gilkey, 1988b).

Although the order of writing data to the computational data base in Figure 5.4 is conceptually correct, when using the CAMDAT file format a modification occurs (Figure 5.5). The input data for the analysis codes (such as mesh and material data) and output results (such as the head, velocity, pathway, and concentration data) are merged. Consequently, because some data are not generated simultaneously, stored data must be read, merged with the new data, and then restored.

Appendix A discusses various aspects of the CAMDAT file format in detail.

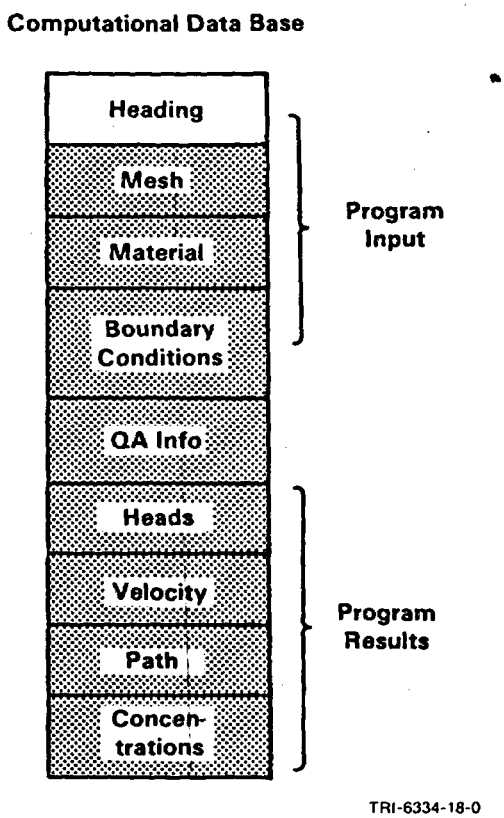


Figure 5.4 Order and types of data stored in a computational data base.

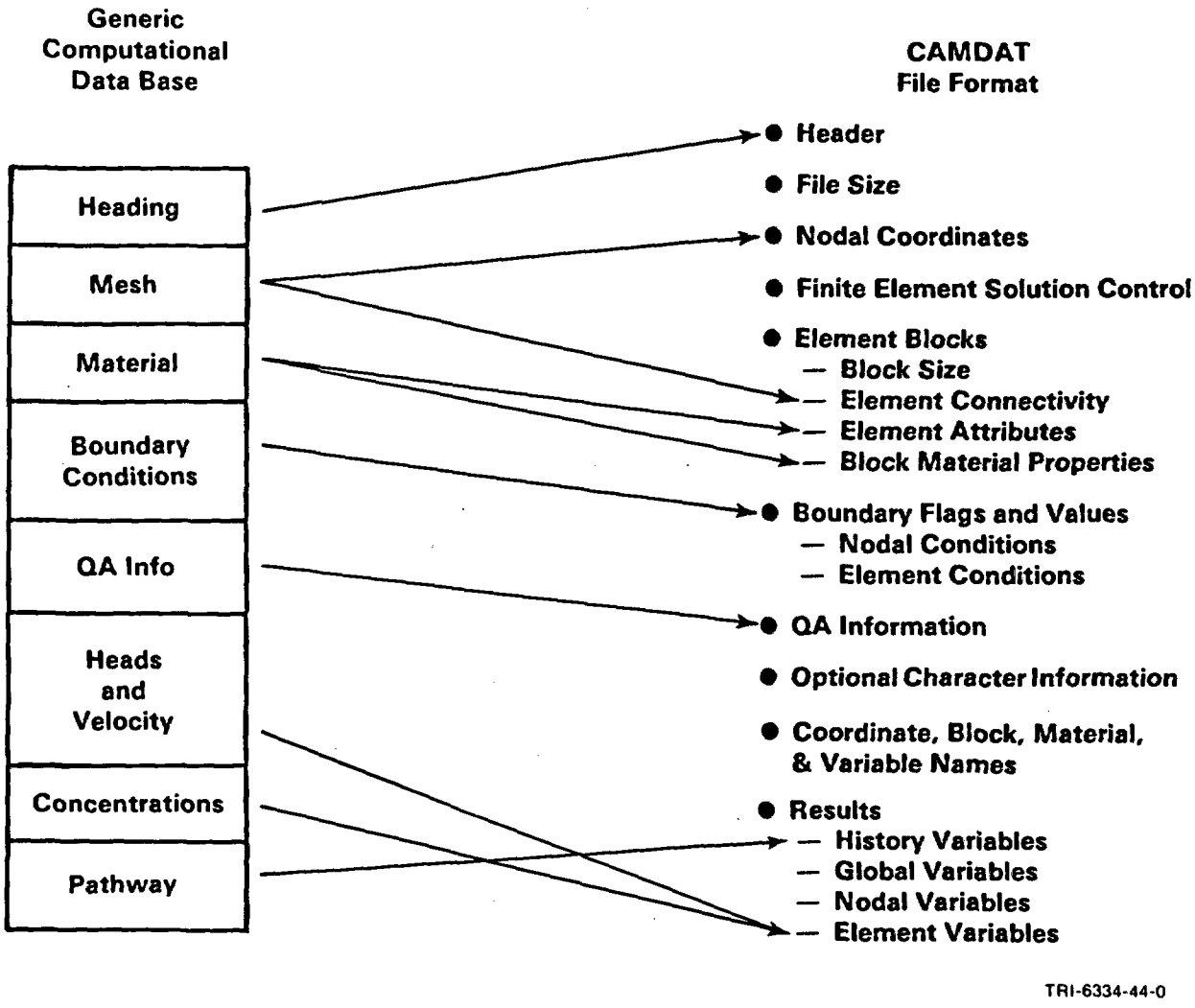


Figure 5.5 Correspondence between generic computational data base and CAMDAT.

6. Code Linkage and Data Flow

This chapter describes the linkage of codes and flow of data controlled by CAMCON during the consequence assessments by dividing the complex flow into a number of small steps, detailed in a number of figures. At the end, the figures are combined to show the complete data flow.

In the following figures and discussion, the computer codes that make up the methodology for assessing compliance are divided into three categories:

- Main modules
- Support modules
- Translators.

Main modules refer to programs that represent major tasks of the consequence assessment. The major headings of this chapter correspond to these main modules.

Support modules refer to codes necessary to facilitate use of main modules. The term support does not refer to size or importance to the overall system algorithm; some of the codes (such as the interpolators) are large and very important to the algorithm. Translator modules refer to codes that translate data either into or out of the computational data base to couple the major and support modules. Necessary support modules and translators are included in the discussion of the main modules.

6.1 Mesh Generation Module

Purpose. The mesh generation module discretizes the three scales of models needed for assessing the consequences of one scenario: the regional hydrologic model, the local hydrologic/transport model, and the repository/shaft model. If the scenario requires other subdomains (e.g., multiple transport paths) additional grids can be included.

Flow of Data. The flow of data for generating a finite-element or finite-difference mesh is from the geometry file of the secondary data base (conceptual model), to a mesh generator, and then into one of the three files of the computational data base, depending upon the model scale (Figure 6.1).

Each main module will probably need additional information (primarily information controlling printout options, etc.). In Figure 6.1, this is depicted by including a "code control" information source supplied by the user in a batch file during setup of a calculation sequence. The code control information will be used directly by the translator to merge with data read from the data base.

Tasks Performed. Once the conceptual model of the disposal system (embodied in the secondary data base) is established in sufficient detail, an analysis of the consequence of a scenario begins. The first task is to convert the conceptual model of a scenario into an acceptable computational model.

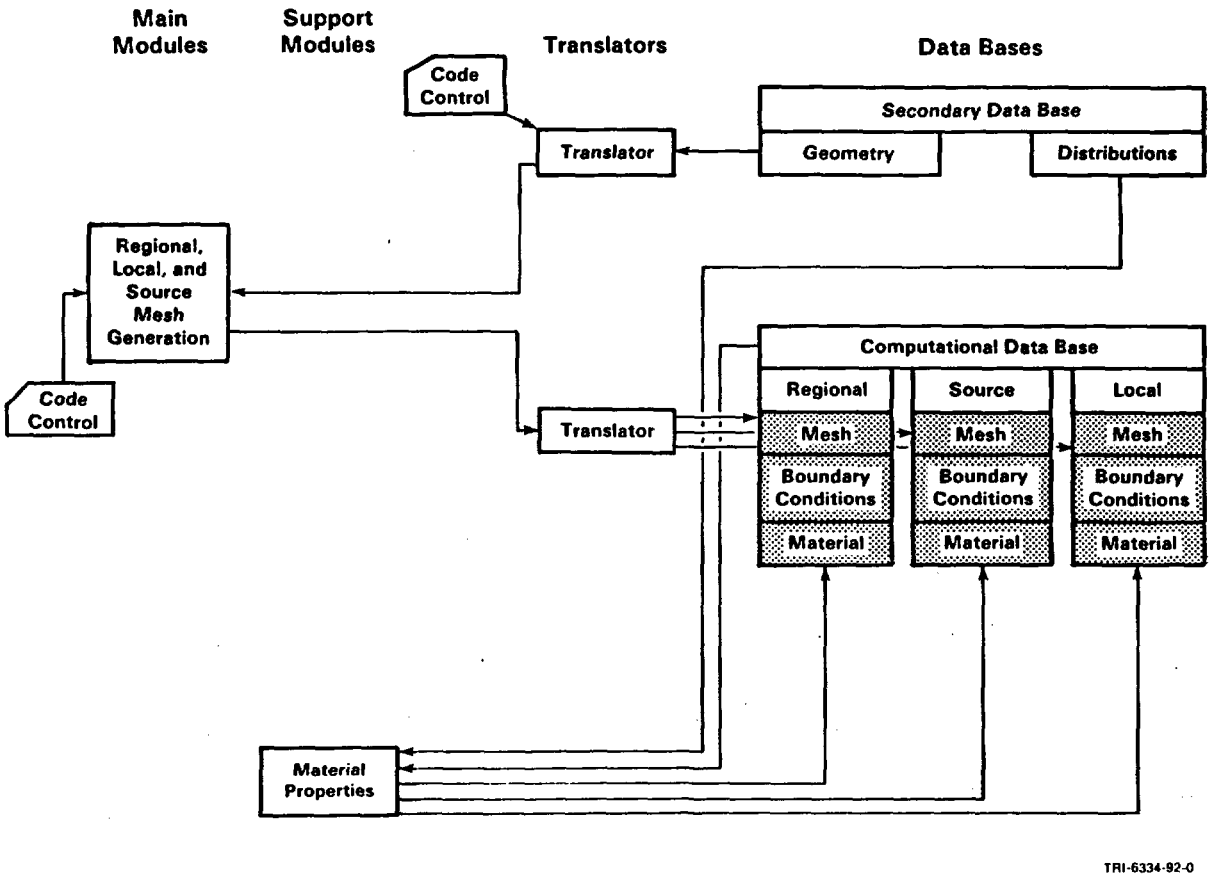


Figure 6.1 Data flows from the secondary data base, to the mesh generator, and then into the computational data base.

Ideally, the mesh generation is separate from the analysis program. This allows an analyst to use generalized and user-friendly mesh generation codes rather than the crude generation programs often attached to analysis programs. Furthermore, because the mesh is stored in a standard file format divorced from the analysis program, only one mesh generator need be used, even though different analysis programs are used to predict results at each of the three model scales: regional, local, and repository.

A finite-element (FE) mesh generator could be used on a finite-difference (FD) grid (or vice versa, although unlikely since it would limit the choice of element grids) by using a computational data base. However, the potential scrambling of node and element numbers when optimizing FE matrices to reduce bandwidth can cause difficulty in translating mesh information stored in the data base to the regular grid numbering required by an FD analysis code.

The locations and flags (IDs) for all boundary conditions are set during mesh generation; thus, Figure 6.1 shows boundary condition data stored in the computational data base after passing through the mesh generation module. Boundary condition values are set by the material support module, material properties, following mesh generation.

Support Module, Material Properties. The material-properties support module inserts into the computational data base user-selected parameter values (often averages) read from the secondary data base. Later, the user may overwrite the values of selected parameters by running the Monte Carlo module.

Application to WIPP. This mesh generation capability is planned for the WIPP, but because much of the numerical model development occurred prior to the implementation of this data flow system, the mesh and boundary condition data for the data base are generated by using a simple translator that reads model geometry information contained in the local and regional model input files.

6.2 Monte Carlo Sampling Module

Purpose. This module samples distributions of input parameters (frequently material or hydrological properties) needed during uncertainty calculations as dictated by *40 CFR 191* and sensitivity analysis. The sampling for the whole system is done at this step (Figure 6.2); thus, the material properties stored are "global."

Flow of Data. This step begins when parameters to be varied are selected from the secondary data base. Following this step, parameter data flow from the distribution file in the secondary data base through a pre-translator for Monte Carlo program setup and then into the Monte Carlo code. The Monte Carlo code generates a specified number of sample vectors, n_v. The post-translator makes n_v-replications of the computational data base (CAMDAT) and inserts one distinct sample vector of the varied parameters into each replication of CAMDAT. Necessary but constant parameters are also extracted from the secondary data base by the post-translator and stored in CAMDAT. These

parameters (constant and varied) are inserted onto each file ("material" in Figure 6.2). Each replication of the data base is then run sequentially through the remaining program modules (Figure 6.2).

Sampling Combinations of Parameters. To maintain consistency, if different combinations of parameters are used in different modules (e.g., some stratigraphic layers are combined in the regional but not in the local hydrologic model), sampling is done on original parameters rather than on combined parameters. Any necessary manipulation of the sampled parameters to obtain code input is performed by a later code translator.

Monte Carlo Sampling for Preliminary and Final Assessments. Figure 6.3 shows the data flow between the mesh and Monte Carlo modules for both the preliminary and the final compliance assessments. Visually, there is no difference between the preliminary and final compliance assessments, but conceptually there is. For WIPP preliminary assessments, the sampling is done individually for each scenario. Conceptually, for final WIPP assessments, the sampling for all scenarios occurs only once prior to evaluating any scenarios. However, provided that the same random number generator with the same seed is used on the same computer, the identical run vectors can be generated very efficiently each time a new scenario is run, rather than actually storing the information. This approach is implied in Figure 6.3.

Application to WIPP. For the WIPP, Latin hypercube sampling (LHS) (Iman and Conover, 1980), an efficient form of Monte Carlo sampling, is used to greatly reduce the number of required samples and to control correlations between parameters. The number of sample vectors required depends upon the number of varying parameters. As a rule of thumb, $n_v \simeq 4/3 \bullet n_\alpha$, where n_v is the number of sample vectors and n_α is the number of varying parameters (Iman and Shortencarier, 1984). The required number of sample vectors, n_v, tends to increase with nonlinear system behavior but tends to decrease as n_α increases.

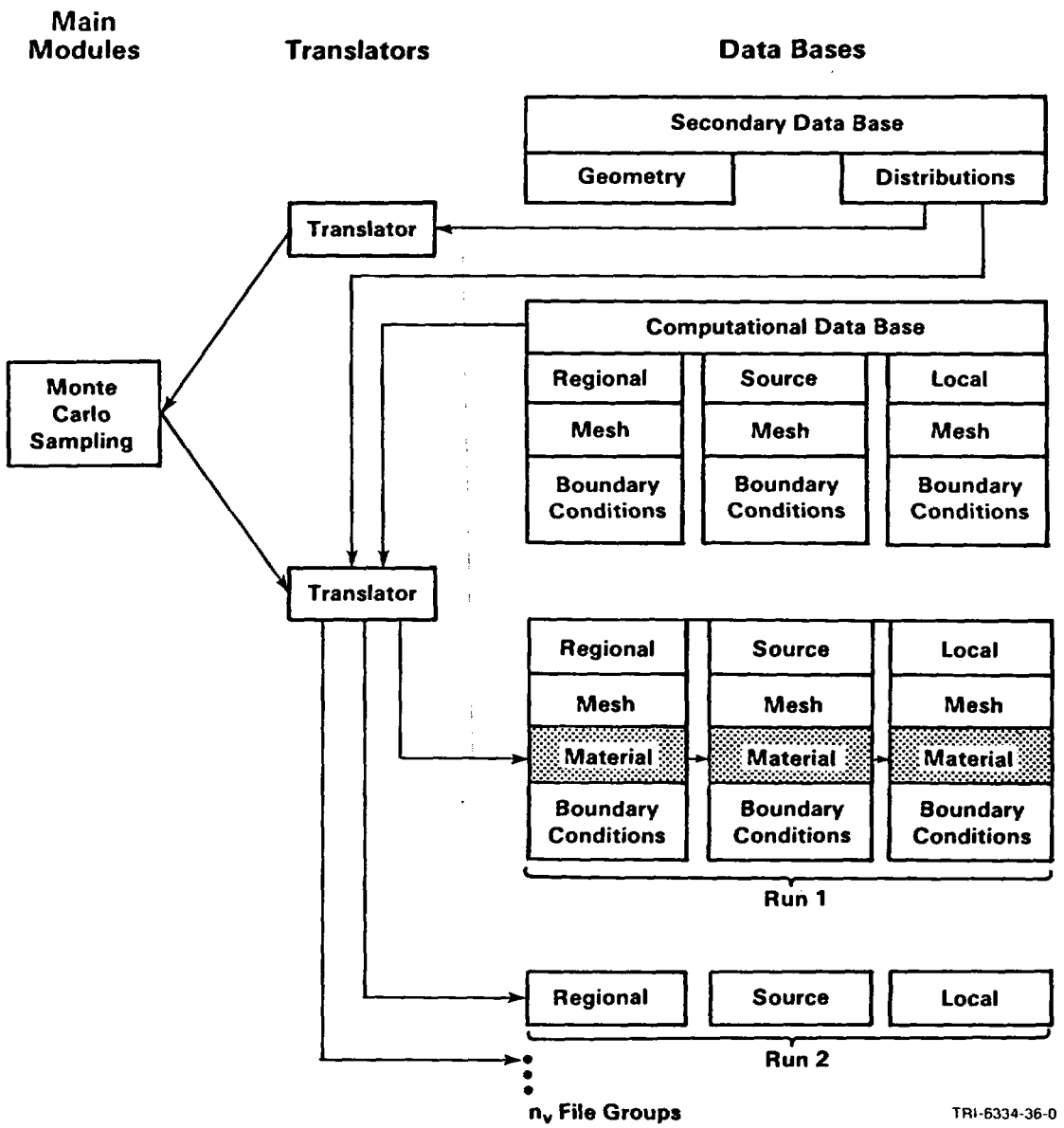


Figure 6.2 n_v-replications of the computational data base result from Monte Carlo sampling.

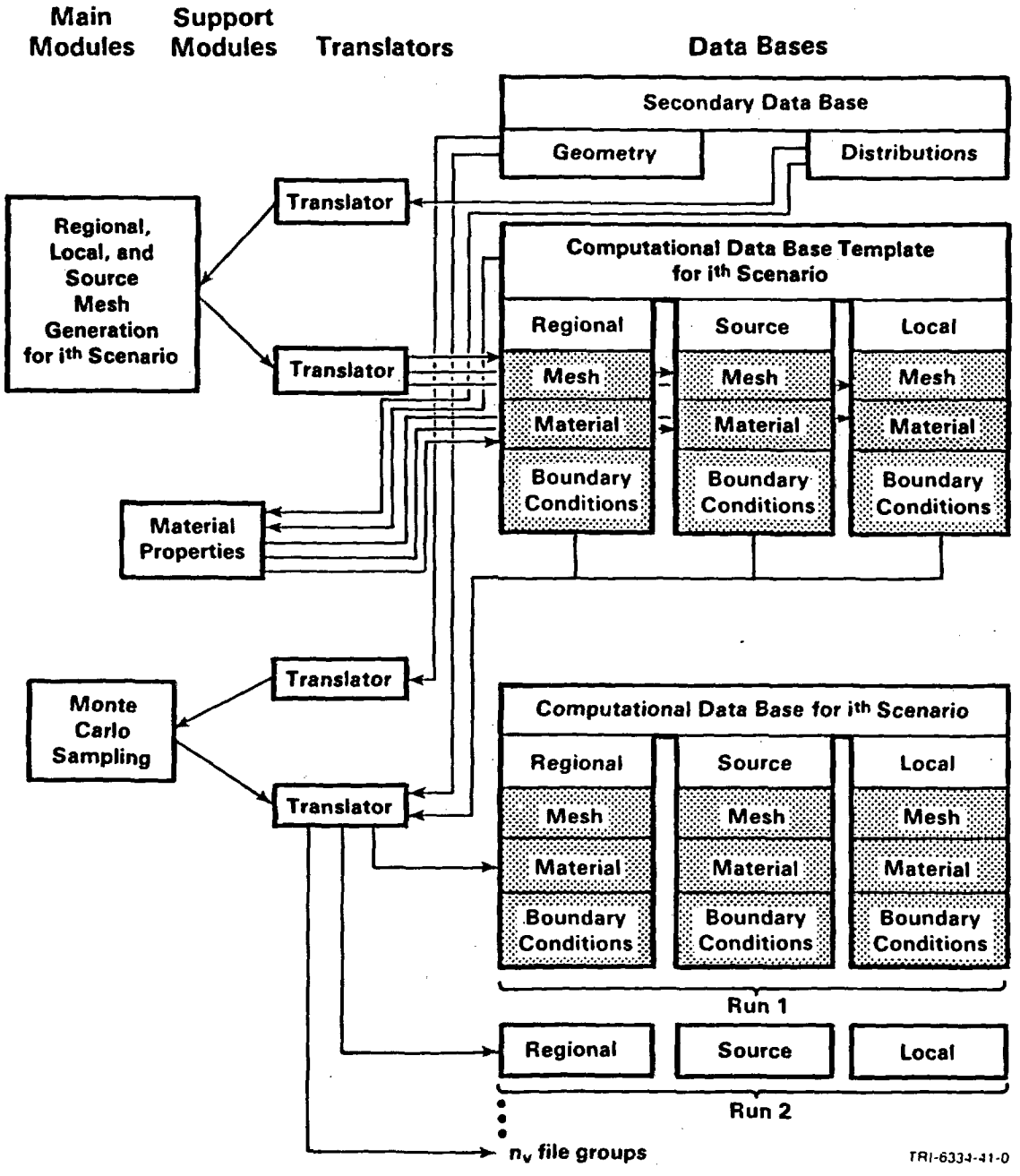


Figure 6.3 Monte Carlo sampling can change material properties set by the material support module.

6.3 Regional Fluid-Flow Module

Purpose. This module calculates the groundwater flow in the region around the repository. Figure 6.4 shows the flow of the data.

Support Module, ALGEBRA. Although not always necessary, a support module, ALGEBRA (Gilkey, 1988a), is shown in Figure 6.4. For many codes not all pertinent data can be generated. Rather than modifying the code to calculate this information and invoking a new quality assessment, the information can be generated external to the program by manipulating data read from the data base and then storing it with previously generated data. As an example, the velocity data are shown being generated from pressure head data (and material property data) already stored in the data base.

Application to WIPP. For the regional model (Los Medanos model) at WIPP, SWIFT II (Reeves et al., 1986) is being used for preliminary calculations and for demonstrating the procedures (Bertram-Howery et al., 1989). The translators written for SWIFT II are fairly specific and do not permit use of all features of this general purpose code. Other codes with the capability to perform transient, variable-density groundwater flow will be examined before a code is selected to use for the final calculations.

The Los Medanos model represents a 30-by-40-km area, with eight vertical layers. The Culebra Dolomite member of the Rustler Fm. is represented by one layer (Brinster, 1989). The Los Medanos model encompasses most of the area originally examined when searching for an appropriate disposal site in southern New Mexico (DOE/EIS, 1980).

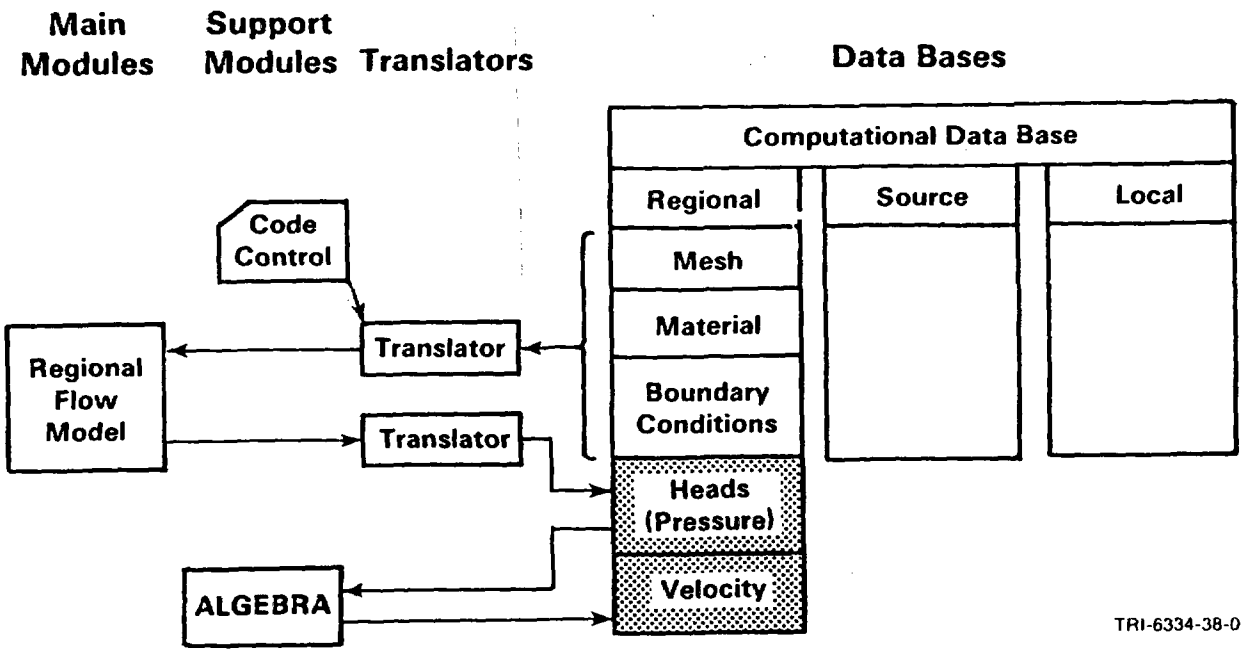


Figure 6.4 Computational data base linked to a regional flow model through translators.

6.4 Local Fluid-Flow Module

Purpose. The local fluid-flow module, a major one in the compliance evaluation, establishes flow conditions within the controlled area for the disposal system.

Flow of Data. Data flow from the regional file of CAMDAT, through an interpolator for defining boundary conditions on the local model, and back into CAMDAT. At this point the local model can be set up using the appropriate pre-translator for the local fluid-flow module (possibly the same as the regional translator if the same groundwater program is used). The velocity and pressure head results are stored in the local model file of CAMDAT after passing through the post-translator of the local module (Figure 6.5).

Interpolating between Model Scales. The local model region, encompassing at least the controlled area, is completely embedded within the regional model; hence, boundary conditions for the local model are prescribed by the regional model. However, occasionally the boundary conditions are established by iterating between the local and regional models as touched upon in Chapter 4. These conditions are established by a support module, "interpolate," using the data stored in the regional model file of CAMDAT (Figure 6.5). The local model boundary conditions are then stored in the local model file.

At this stage of the calculations, compliance with the NRC groundwater travel-time requirement can be assessed (see Figure 3.5) (unnecessary for the WIPP).

Application to WIPP. For the local model at the WIPP, SWIFT II (Reeves et al., 1986) is being used for preliminary calculations and for demonstrating the procedures (Haug et al., 1987). Consequently, the same translators used for the regional model are used here.

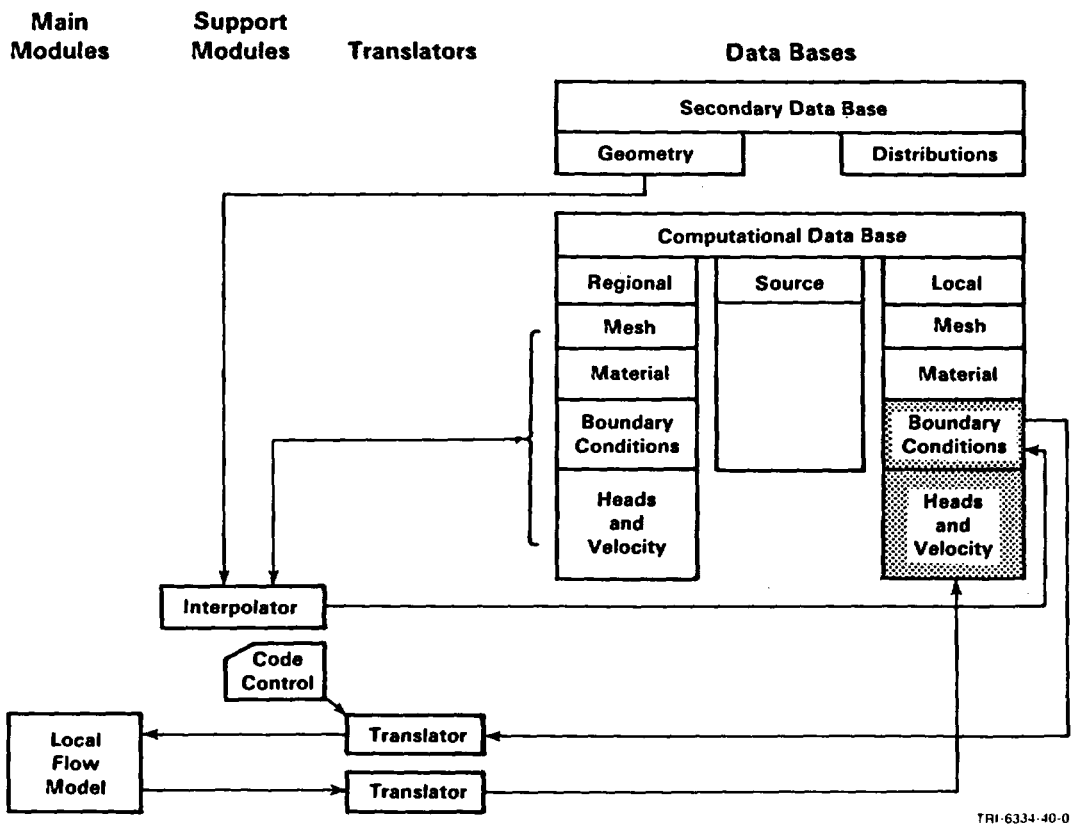


Figure 6.5 Interpolation module sets local model boundary conditions.

6.5 Repository/Shaft Module

Purpose. This module calculates brine flow and radionuclide transport within the repository and access shaft. It includes complex processes in the storage room, panel seals, drifts, shaft, and shaft seals. The source term is within the storage room part of this systems model.

Flow of Data. The flow of data is similar to that for linking the local fluid-flow module. The only difference is that data originate in the local file of CAMDAT rather than the regional file, and end up in the source file of CAMDAT rather than in the local file (Figure 6.6). Specifically, fluid-flow conditions from the local model define boundary conditions for the repository model using a support module, "interpolate." Then the repository model is set up using the appropriate translator. Concentration results are stored in the repository file of the data base.

A subtle difference can occur, however, when groundwater enters the repository from human intrusion (e.g., drilling that penetrates the repository and then a pressurized brine pocket). In the human intrusion scenario, additional conditions for the groundwater inflow are required.

At this stage of the calculations, compliance with the NRC's two engineered barrier requirements can be assessed (see Figure 3.5). Presumably, the waste package submodel of the storage room would be used for the waste package release rate. This evaluation is unnecessary for the WIPP.

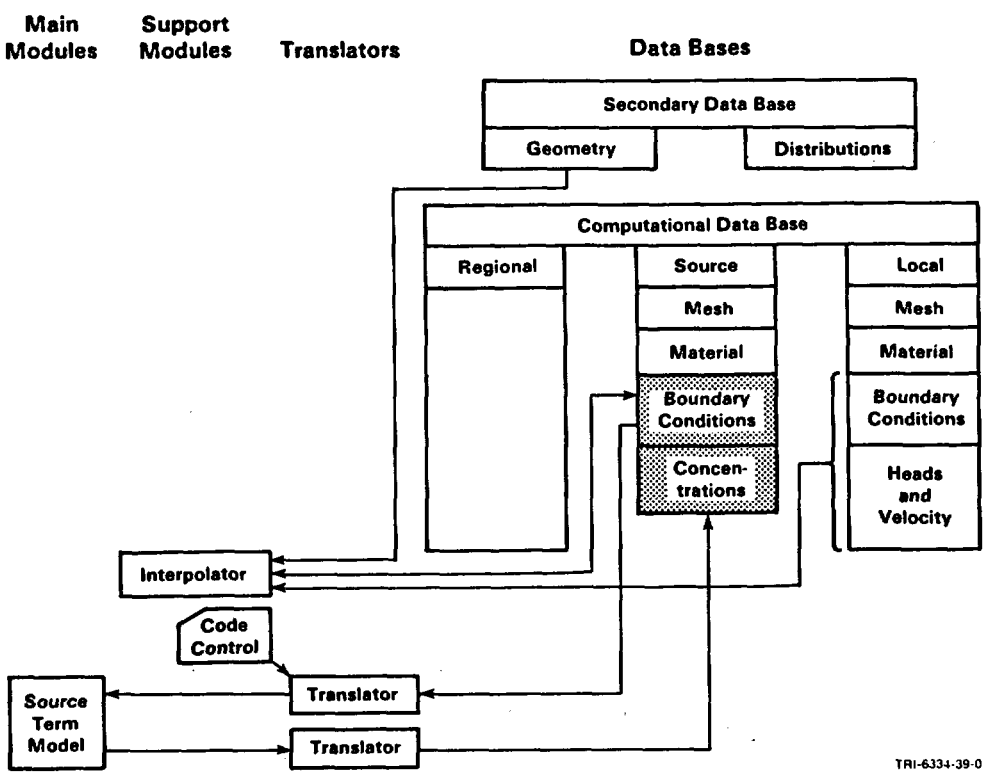


Figure 6.6 Source concentrations found from repository model after interpolating boundary conditions from local model.

6.6 Nuclide Transport Module

Purpose. This module predicts radionuclide migration from the repository source to the targets of interest: the accessible environment boundary for the Containment Requirements, a special source of groundwater for the Groundwater Protection Requirement, or the public for the Individual Protection Requirement.

Methods. Three methods exist to predict transport: (1) coupled hydrology/transport calculation from the entire domain, (2) transport calculation for a subdomain, using detailed code, or (3) transport calculation for a subdomain, using a simple conceptual model analytically solved along the trajectory of a neutrally buoyant particle, the "pathway" (e.g., the Network Flow and Transport Program, NEFTRAN [Longsine et al., 1987]).

The latter two cases reduce the computational burden by first establishing the predominant nuclide pathway using a support module, "tracker" (Figure 6.7). The tracker module estimates particle movement from a specified origin by calculating movement along the maximum velocity gradient. Along this particle pathway, a subdomain of the local model can be used for radionuclide transport calculations.

One of the goals of a sensitivity analysis (performed early in the compliance assessment) is to help the analyst choose the proper method for the transport calculations.

Flow of Data. Assuming that the local model encompasses the controlled area, the velocity field of the local model is used by tracker to specify a pathway. This pathway can be used to establish a reduced computational domain from the transport module, if necessary. The velocity field, and source-term concentrations and pathway (if using a subdomain) are then accessed by the pre-translator for the transport module. After passing through the post-translator, transport calculation results are then stored in the local file of CAMDAT (Figure 6.7).

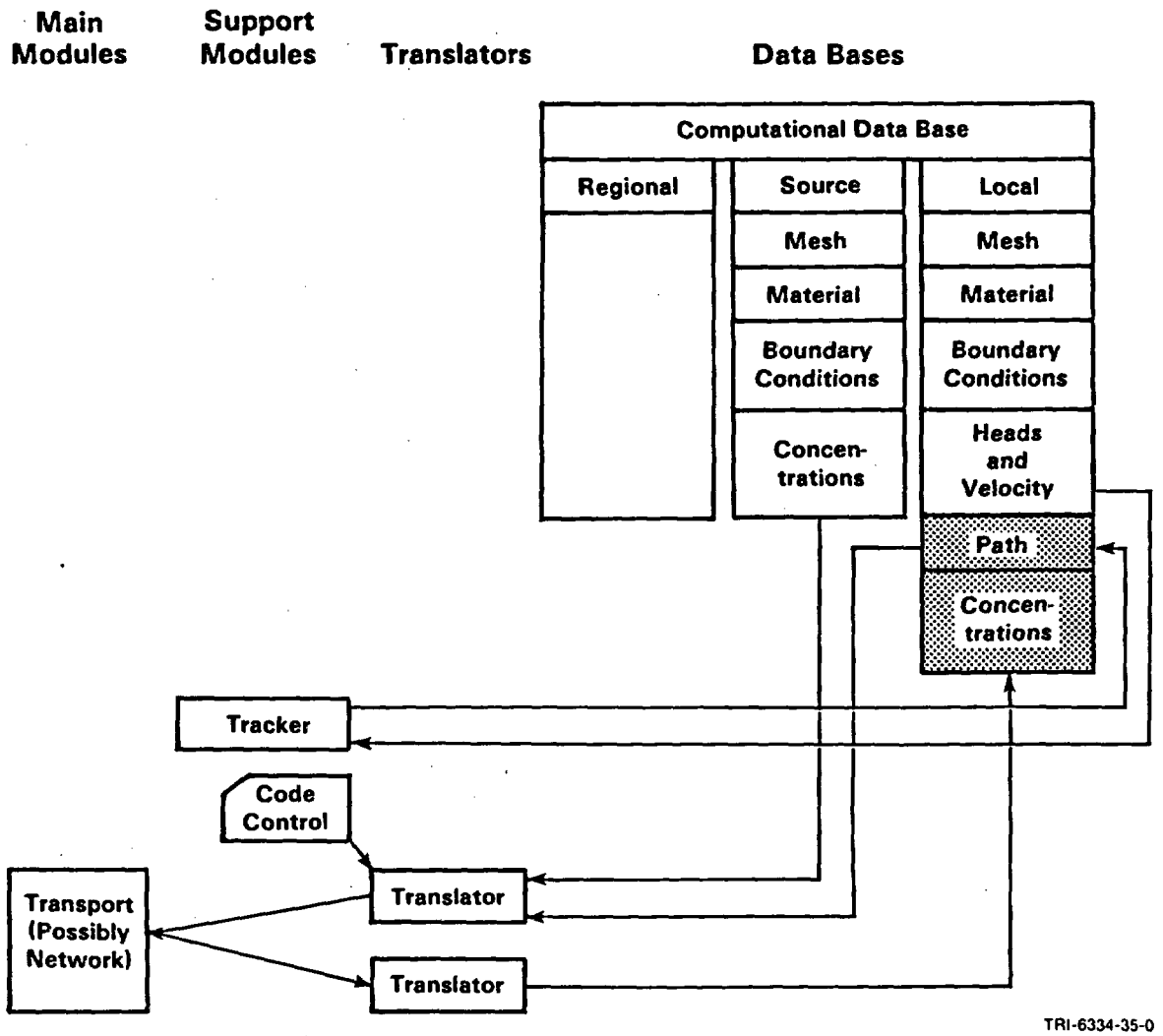


Figure 6.7 Transport calculations made using repository and local model information.

6.7 Plotting Module

The plotting support module (Figure 6.8) plots all intermediate and final results from the main modules. Although it is discussed near the end, results can be displayed at any time because a neutral file format, CAMDAT, is used throughout the consequence assessment. For the WIPP, the plotting package BLOT (Gilkey, 1988b) (a combined version of DETOUR [Gilkey and Flanagan, 1987], SPLOT [Gilkey, 1986a], and TPLOT [Gilkey, 1986b]) is used. It directly reads the CAMDAT data base, making a translator unnecessary.

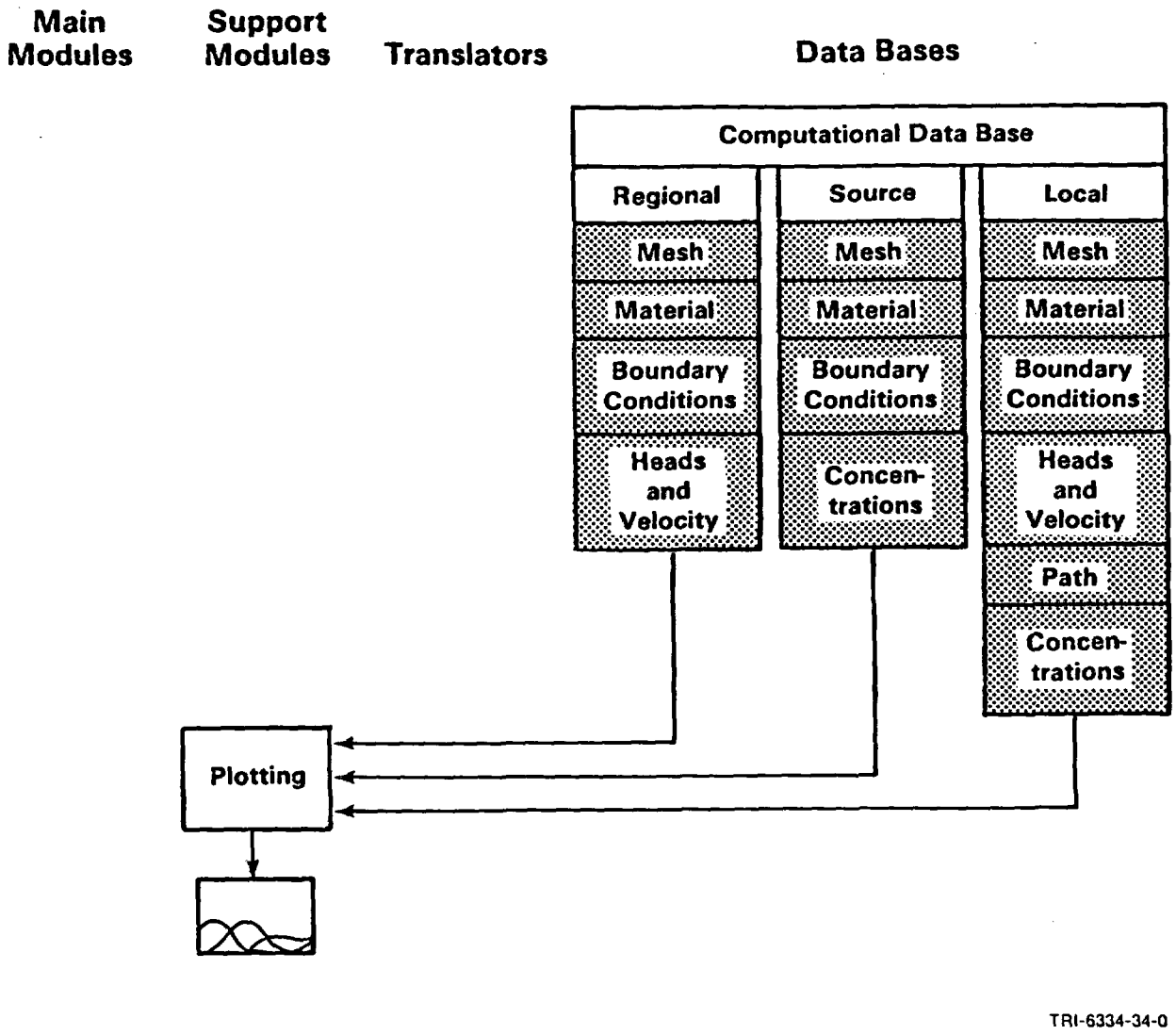


Figure 6.8 Results can be displayed throughout computations when using computational data base.

6.8 Final Calculations

At this stage of the compliance assessment calculations, different paths are taken, depending upon which of the three EPA requirements are being evaluated (this divergence of calculation paths is shown in Figure 2.3).

Containment Calculations. To assess compliance with the containment requirements, the data flow steps described above are repeated for each of the simulations, n_v, for any one scenario. Then the steps are repeated again for the n_s scenarios compiled for the disposal system. Thus, when the containment assessment calculations are complete, $n_s \bullet n_v$ simulations have been run.

For the containment requirement, the final calculations must use the results from all the simulation runs, nv, on all the scenarios, ns, to generate the CCDF for comparison with the Containment Requirements (*40 CFR 191.13*) (Figure 6.9). Generating the CCDF requires

- Evaluating the total (integrated) discharge over 10,000 yr, using release results (e.g., release versus time for each radionuclide)
- Calculating EPA sums
- Multiplying by the scenario probabilities.

All these calculations are performed by the final main module, CCDF generation (Figure 6.9).

Although only the final release results appear to be necessary, all data in these simulations are saved at first (Figure 6.9). The primary reason is that the importance of any one scenario or simulation is unknown until the results have been combined. Critical examination of the scenarios and subsequent modeling may be required to explain unexpected behavior or even compliance violations. After documenting all results, data may be destroyed, provided that the QA information in the files is retained to allow reconstruction of the data, if necessary.

Groundwater Concentration and Dose Calculations. To evaluate compliance with the Individual Protection Requirement (*40 CFR 191.15*) and the Groundwater Protection Requirement (*40 CFR 191.16*), the analyst must calculate radionuclide concentrations. The undisturbed performance scenario (scenario excluding human intrusion and other unlikely events) is used for these calculations. Compliance with *40 CFR 191.16* can be evaluated after performing the transport calculations if a "special" source of groundwater exists (none exists at the WIPP site [WIPP Strategy, 1988]). Evaluating compliance with Individual Protection Requirements (*40 CFR 191.15*) requires that the analyst replace the CCDF module with the biotransport and dosimetry module shown in Figure 6.10. No release in the first 1,000 yr is anticipated at WIPP, but the biotransport and dosimetry module is being prepared as a contingency.

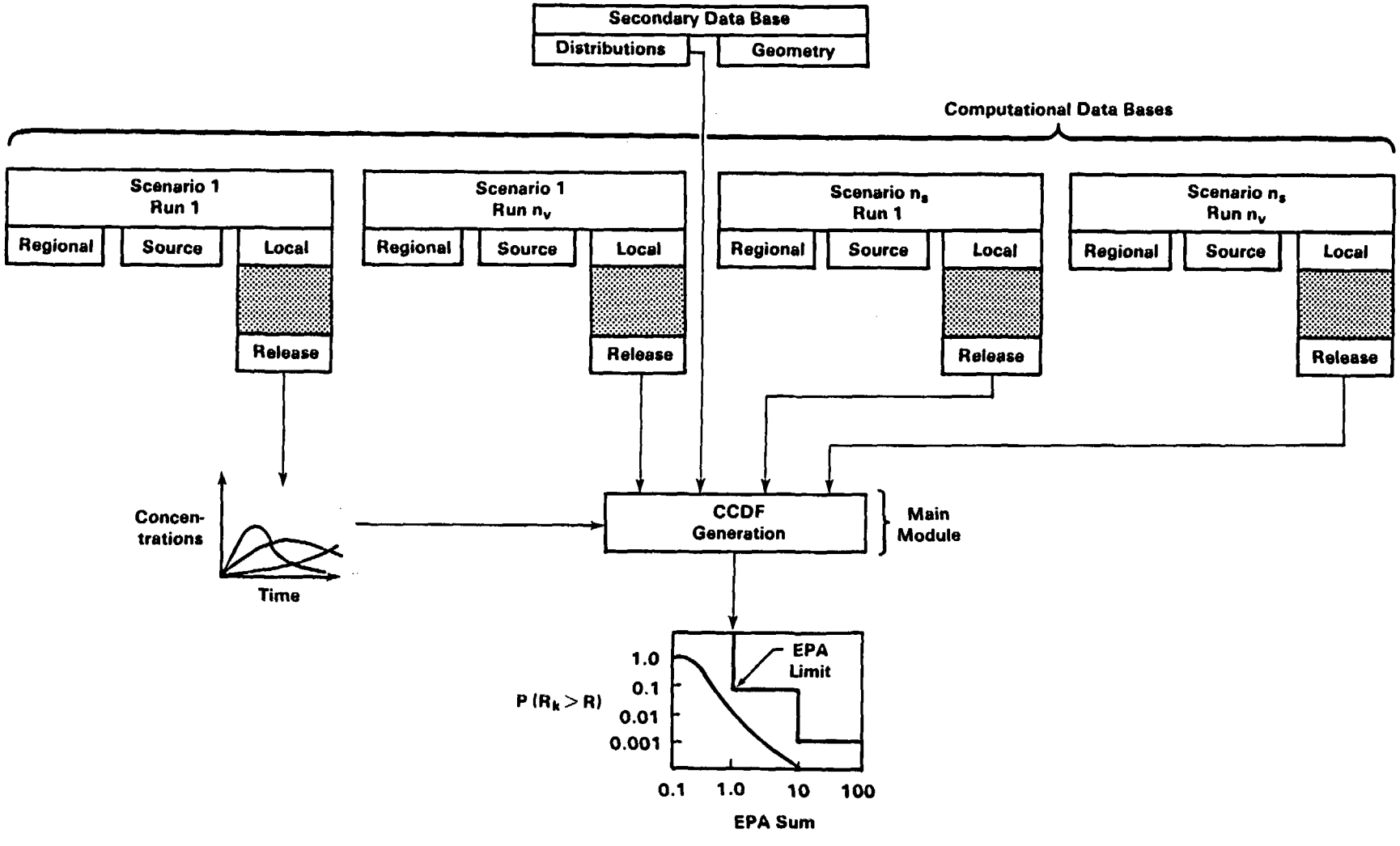


Figure 6.9 The final task combines release results from $n_s \bullet n_v$ runs to generate a CCDF for comparison with EPA Standard (*40 CFR 191.13*).

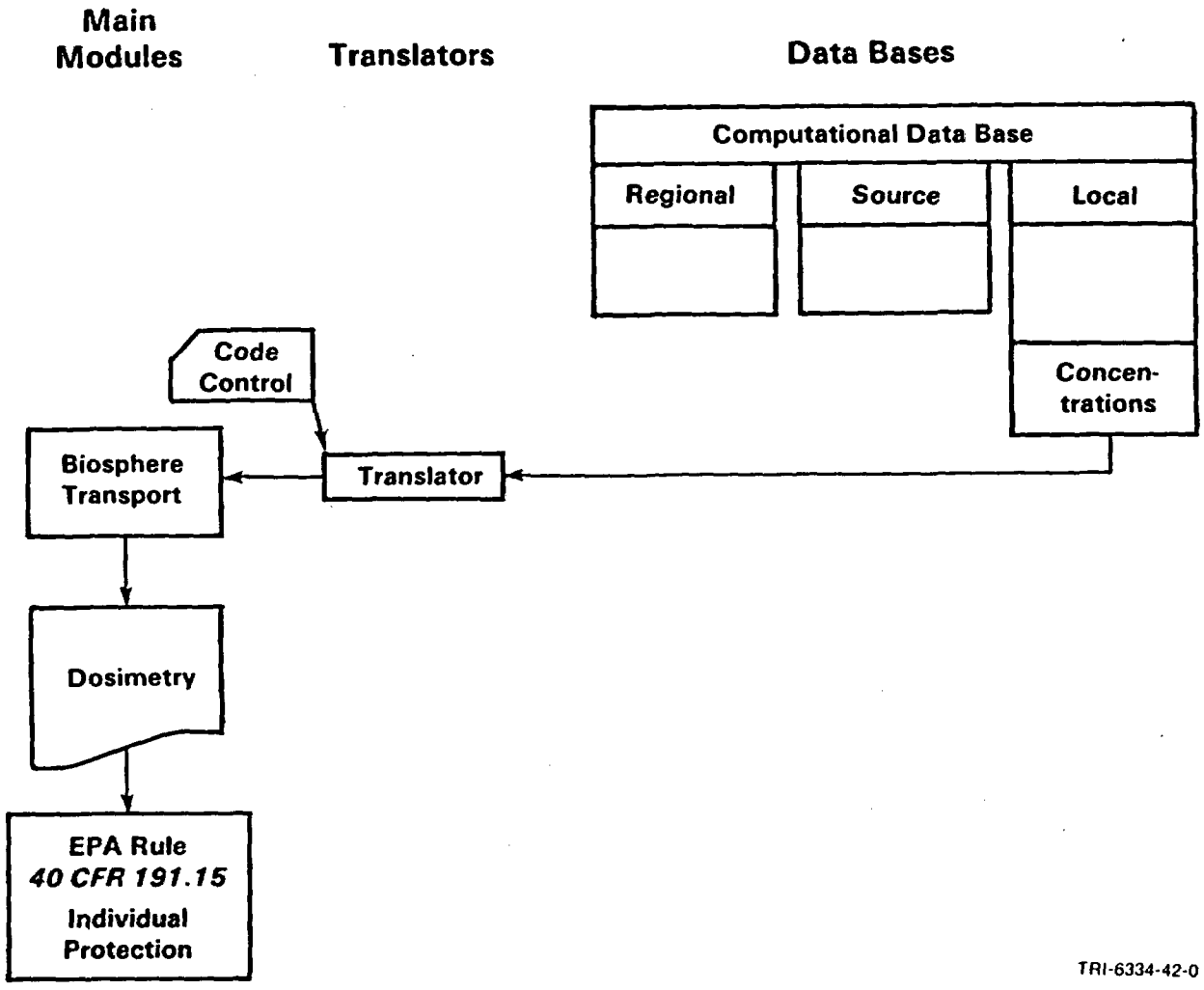


Figure 6.10 Biosphere transport module used with undisturbed scenario to assess compliance with individual protection requirement (*40 CFR 191.15*).

6.9 Summary of Data Flow

Figure 6.11 shows the algorithm used for assessing consequences of scenarios for deep geologic repositories. It summarizes Figures 6.1 through 6.9. The data flow is complex for consequence assessment, necessitating a logical data flow. This data flow is aided by using CAMDAT. Having logical data flow between CAMDAT and the various program models makes constructing a data flow controller, CAMCON (Rechard, 1989), relatively easy.

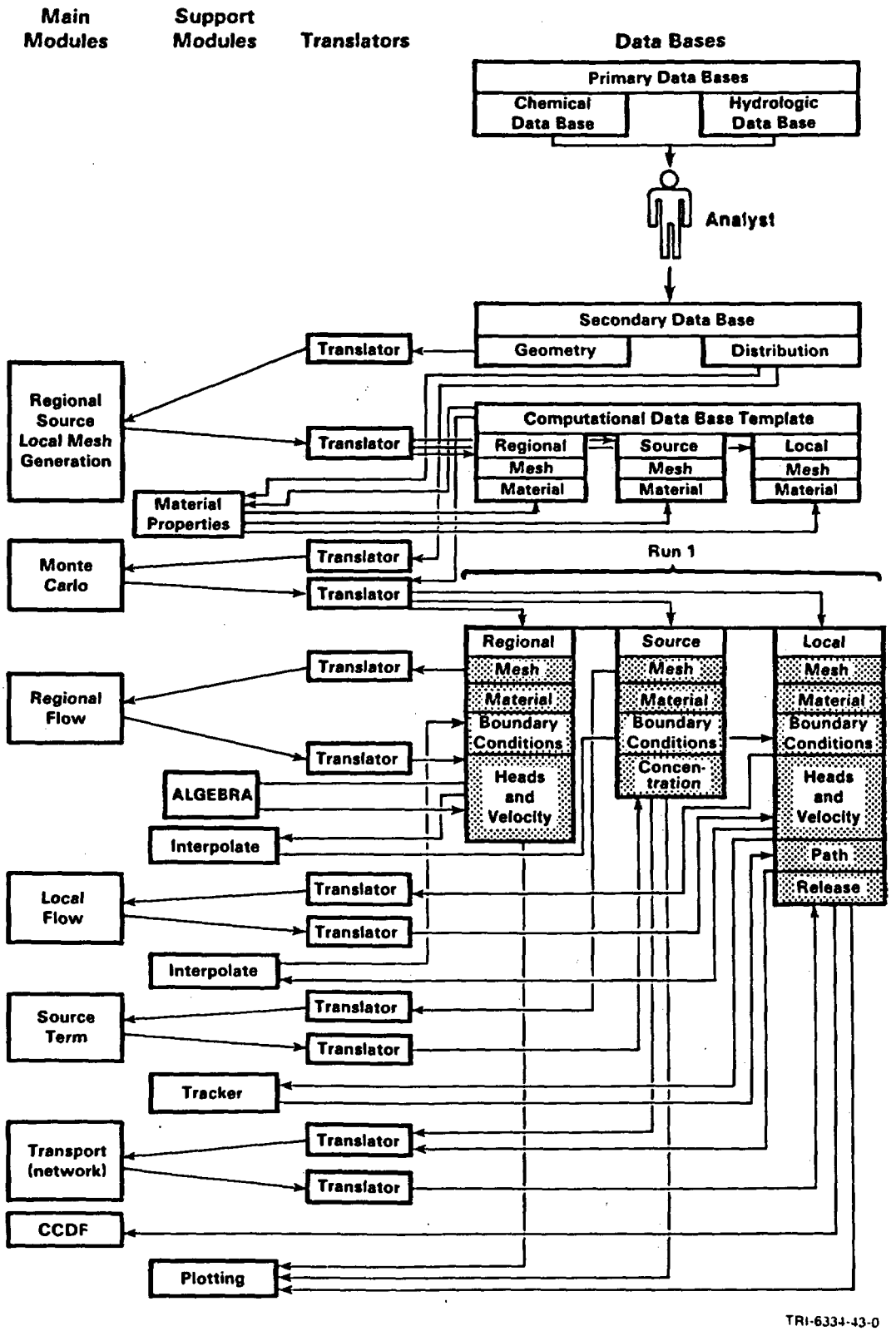


Figure 6.11 Data flow in consequence assessments is complex; careful data control is necessary.

Appendix A: Computational Data Base, CAMDAT

The purpose of Appendix A is to

- Describe the CAMDAT computational data base file format (file designated CAMDAT Sxx_t.CDB for WIPP)
- Specify the file format, using a FORTRAN code fragment.

The descriptions of CAMDAT reiterate information pertinent to the WIPP project reported by Taylor et al. (1986) and Mills-Curran et al. (1988) concerning the GENESIS and EXODUS data base after which the computational data base is designed.

A.1 General File Format Description

For the WIPP both finite-element (FE) and finite-difference (FD) numerical analysis information has to be accommodated. The file format was originally designed for FE information; hence, the file structure described below uses FE terminology. However, the structure can easily handle FD analysis information as well, except that a few terms must be interpreted somewhat differently by the analysis codes. For example, although the definition of the term "nodal point" changes between FE or node-centered FD and body-centered FD analyses, for the WIPP a node is always described as in FE analysis to be consistent (Figure A.1). Although not limited by CAMDAT, the node and element numbering used for WIPP FD grids is also shown in Figure A.1.

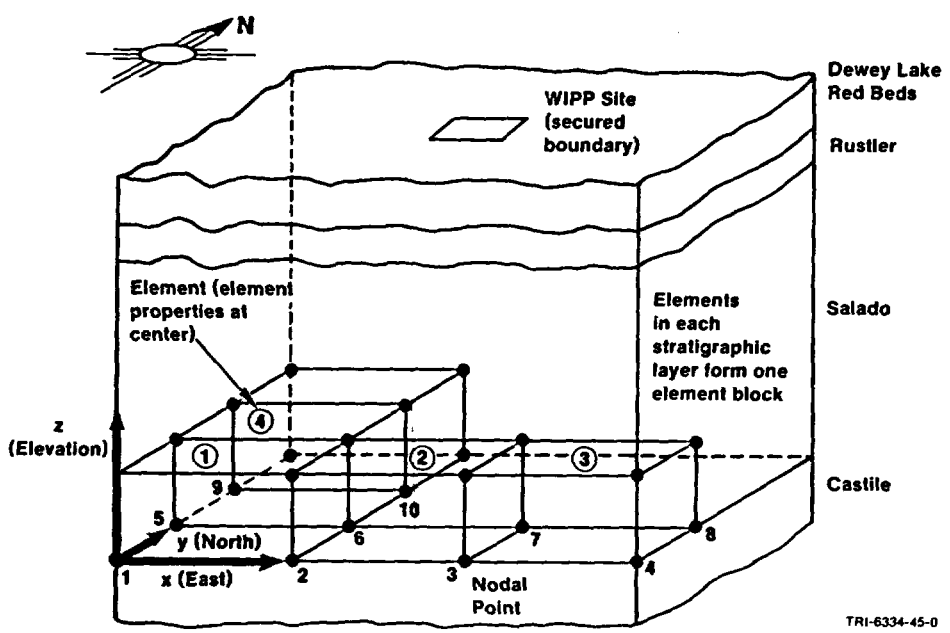


Figure A.1 Storage of WIPP finite-difference mesh in CAMDAT.

A description of each file component follows. With much of the file format, variations in interpretation of the data in each record can occur if a consistent convention is used between analysis codes that access the data.

A.1.1 **File Format.** The CAMDAT file format possess three general features:

- File is structured so that the length of all records is defined before the record is read, implying that the reading program can dynamically allocate memory for all arrays
- File uses a sequential file format to keep the file structure simple and easy to use for programmers
- File stores data as unformatted binary for space efficiency.

For example, see the OPEN declaration in the FORTRAN segment (Section A.2).

Although binary storage greatly reduces storage requirements, it limits the direct use of the file on dissimilar computer systems. The usual approach is to either to develop a binary translator (possible because the file is very structured) or have all programs (or do all data base access) on one system. The latter approach is being used at SNLA.

The default unit numbers for the computational data base files are:

- NCDB = 31 for the file storing regional scale data
- NCDB = 32 for the file storing source (repository) scale data
- NCDB = 33 for the file storing local scale data.

A.1.2 **Heading.** The first record is an 80-character string placed on all printouts and plots from the computational data base. For the compliance evaluation, the following four groups of data (separated by commas) are recorded on this line:

1. IDSCNR - succinct scenario ID (CHARACTER*8)
2. SCLMTH - scale of the computer model (CHARACTER*8); choices are REGIONAL, SOURCE, or LOCAL
3. SIMRUN - the simulation run number (CHARACTER*8)
4. TITLE - descriptive, but brief title for stored data (CHARACTER*56).

A.1.3 **File Sizing Parameters.** The ten integers of the second record define the size of most arrays stored in the file. The following parameters are read:

- Geometric information
  1. NUMNOD - number of nodes (either FE or FD)
  2. NDIM - number of coordinates (spatial dimensions) per node
  3. NUMEL - total number of elements, including all element types

4. NELBLK - number of element blocks (for compliance evaluation, NELBLK is the number of different materials)

- Boundary condition information (discussed later in Section A.1.7)

5. NUMNPS - number of nodal point sets
6. LNPSNL - length of the nodal point sets node list
7. NUMESS - number of element side sets
8. LESSEL - length of the element side sets element list
9. LESSNL - length of the element side sets node list

- Data base version

10. NCDBVR - version number of data base (QA feature--programs accessing the data file abort if NDBVER does not equal the assumed version number in the program).

A.1.4 Nodal Point Coordinates. All nodal point coordinates are contained in the third record. The coordinates are read by layers; that is, the node number cycles faster than the x,y,z-component. The labels for the x,y,z-component are specified later in the file with all the block and variable names.

A.1.5 Optimized Element Order Map. The fourth record contains a mapping defining the order in which elements should be processed by a wavefront solver. Because the codes used in the WIPP compliance evaluation do not require this information, it is skipped with a null read statement.

A.1.6 Element Block Information. Element (or grid block) data are stored in blocks or groups. Each block has the same material and element type. Grouping elements with similar material and element type is more space efficient and permits vector processing of each element block. The number of an element is implicitly defined by the order in which it appears in the file. Elements are numbered consecutively across all element blocks. Three records exist for each element block as described below.

A.1.6.1 *Element Block Sizing Parameters.* The first record in each block contains a block ID and four parameters that define the size of all arrays:

1. IDEBLK - unique integer identification (ID) for this element block
2. NUMELB - number of elements in this block (sum of NUMELB for all blocks equals NUMEL)
3. NELNOD - number of nodes defining the connectivity for this element
4. NATRIB - number of attributes for this element type
5. NUMPRP - number of material properties for this block.

Both element and block-specific information can be stored in the file format. The element attributes can change with each element. The block data refer to groups of elements representing different types of materials or layers of strata surrounding the repository. By assigning a unique ID to the blocks, an analysis

code can decipher the order in which materials or layers are stored in the computational data base. Although some material properties are stored as block information, many are stored as element attributes to accommodate subtle changes of parameters within the same stratigraphic layer, if necessary. Consequently, both types of storage are used for the WIPP.

The FORTRAN fragment shown later assumes that the information in each block is read and processed, and that pertinent data are stored in other variables; consequently, an index is not shown for the variables. Frequently, a program accessing the data file may choose to index the variables (IDEBLK(k), NUMELB(k), etc.).

A.1.6.2 *Connectivity for this Element Block.* For FE analysis, the nodes connected together to form each element are stored in this record. No convention is specified in the data base, which implies that the codes must agree on conventions. For the codes used at SNLA, a counterclockwise ordering of nodes is used to define elements. In addition, for three-dimensional analysis, node numbering begins at the far face and ends at the near face with node 5 in front of node 1.

For FD analysis, the connectivity is unnecessary; however, at SNLA an FE plotting package is used to display results for both the FE and FD analysis so that an analyst has to learn and use only one plotting package. In this instance a connectivity array is necessary for the FD results as well, but the array is very regular.

A.1.6.3 *Attributes for each Element and Material Properties of this Element Block.* The third and final record for each element block contains supplementary information for each element and/or the element block (no conventions are specified in the file format, but the arrays allow programs accessing the data base to decipher the parameters stored).

The attribute array, ATTRIB(natrib,numelb), stores information pertaining to properties that vary with each element (e.g., structural beam elements, which require cross-sectional properties). The material property array, XMATPR(numprp), stores information pertaining to properties that vary with each element block.

For the WIPP compliance evaluation, both sampled and constant material properties (~25) were stored in the data base. Because of the constraints finite-difference codes pose when modeling the irregular geometry of stratigraphic layers (e.g., layers pinching out), many material properties (e.g., hydraulic conductivity, brine densities) are stored in the ATTRIB array. This storage scheme allows properties to vary within one stratigraphic layer (defined as an element block). As mentioned earlier, this storage scheme is also important for storing trends. Data known to not vary or vary only slightly (e.g., porosity, rock density, nuclide partition coefficients) are stored in the XMATPR array.

A.1.7 **Boundary Condition Data.** The file format can store boundary condition information (e.g., load or fluid pressure conditions) in two ways:

- Node point sets
- Element side sets.

The original interpretation of the records is described below. Variations in the interpretation of the data contained in each record did occur for WIPP.

A.1.7.1 *Node Point Sets.* A node point set refers to a set of nodes (one or many) that has been identified with a unique ID (flag). Although a particular node may appear in any number of node sets, a node should appear only once in each node set. Each node in a set is assigned an individual factor (e.g., pressure or flux). All nodes sets are concatenated into one list; similarly, distribution factors for all nodes are concatenated. Consequently, besides the IDs, the node set lists distribution factors; a pointer list and a counter list are required. These five data components (four integer lists and one real data list) are recorded on five separate records. Their description follows.

A.1.7.1.1 IDs for each nodal point set. The first nodal point set record contains the ID (flag) and an eight character identifier of each node set. Similarly to the element block ID, the node set ID is a unique integer label assigned by the user. The record length is 2 x NUMNPS, which is the fifth parameter defined in Section A.1.3.

A.1.7.1.2 Number of nodes in each nodal point set. The second record of the nodal point set data contains the number of nodes (integer) in each node set. The length of this record is NUMNPS.

A.1.7.1.3 Pointers for locating each nodal point set. The third record contains an integer pointer for each node set which locates the beginning of the node set within the concatenated node list contained in the fourth record. The length of this record is also NUMNPS.

A.1.7.1.4 Concatenated list of nodal point sets. The fourth record contains the lists of nodes (integer) for all sets concatenated into a single list. The count and pointer lists in the previous two records are used to identify the nodes in any particular node set. The record length is LNPSNL, the sixth parameter defined in Section A.1.3.

A.1.7.1.5 Factors corresponding to each nodal point. The fifth and final record of the nodal-point set data contains a concatenated list of nodal factors. Depending on how the analysis program interprets the data, these factors either prescribe the actual constraint conditions (e.g., pressure or flux) or the spatial distributions of the constraints (interpreted as multiplication factors). The record length is LNPSNL.

A.1.7.2 *Element Side Sets.* An element side set refers to a set of elements identified with a unique ID. This feature is useful for surface boundary conditions (e.g., heat or fluid flux).

Similarly to nodal point sets, an element side should appear only once in each element side set. However, the element number may appear more than once within a side set if more than one side of an element is part of the set. Further, the nodes associated with a side set will generally appear several times

within that side set's node list. Likewise, each side in a set is assigned an individual factor (e.g., flux). As before, all side sets are concatenated into one list; in the same way, the factors for all side sets are concatenated.

Consequently, the required information for storing element side sets is similar to that for storing nodal set data (IDs, counts, pointers, nodal list, factor list), except that both the element side and the element side's associated nodes must be stored. Consequently, eight data components exist: one ID list, two count lists, two pointer lists, one element side list, one nodal list, and one factor list. These eight data components (seven integer lists and one real data list) are recorded on eight separate records. Their description follows.

For the WIPP, the finite-element codes use arrays as described. The finite-difference codes need only a few of the arrays because nodes associated with an element are easily deciphered, since the mesh connectivity is regular.

A.1.7.2.1 IDs for each element side set. The first data record of the element side set contains the ID (flag) and an eight character identifier of each side set. The record length is 2 x NUMESS, the seventh parameter defined in Section A.1.3.

A.1.7.2.2 Number of element sides in each element side set. The second record is an integer array containing the number of element sides in each side set. Similarly to nodal point sets, an element side should appear only once in each element side set. The record length is NUMESS.

A.1.7.2.3 Number of nodes associated with each element side set. The third record contains the total number of element side nodes in each side set. The number of nodes per element side is implied by the type of element (e.g., quadrilateral). The record length is also NUMESS.

A.1.7.2.4 Pointers for locating elements associated with the side set. The fourth record contains the pointers for locating each set of elements comprising the element side set within the concatenated list of elements for the side sets. The record length is also NUMESS.

A.1.7.2.5 Pointers for locating nodes associated with side set. The fifth record contains a pointer to locate the set of nodes associated with each side set within the concatenated list of all nodes. The record length is also NUMESS.

A.1.7.2.6 Concatenated list of elements encompassing all side sets. The sixth record contains a concatenated list of elements encompassing all side sets. The record length is LESSEL, the eighth parameter defined in Section A.1.3.

A.1.7.2.7 Concatenated list of nodes encompassing all side sets. The seventh record contains a concatenated list of nodes encompassing all side sets. The record length is LESSNL, the ninth parameter defined in Section A.1.3.

A.1.7.2.8 Concatenated list of factors for nodes comprising side sets. The eighth and final record of the element-side-set data is a concatenated list of nodal factors (real). This list corresponds one-for-one to the concatenated list of nodes of Section A.1.7.2.7; consequently the record length is LESSNL.

A.1.8 **Quality Assurance Information.** The first record of this block of data stores the number of quality assurance records (NQAREC)--a value which changes each time a code writes to the file. The next NQAREC records store the eight-character name, version, date, and time of all codes that write to the file (e.g., LHS, 1.0 VAX, 10/1/88, 09:30:00). This information assures that the calculations can be repeated--an important function of quality assurance procedures. Along with the HEADER record, the name, version, date, and time of each code that writes to the file are printed on all plots or printouts of data from the data base.

A.1.9 **Optional Text.** The next segment of the file stores any number of records of optional text. The first record of this segment stores the number of optional records (NXINFO). The following NXINFO records store optional text as CHARACTER*80.

For the WIPP compliance evaluation, the first record stores the random seed, SEED, as a character variable for Monte Carlo sampling.

In addition, for the WIPP, the translators for finite difference codes frequently require the number of elements (computational cells or grid blocks) in the x, y, and z directions. Although the information could be computed each time, the information (NX, NY, and NZ) is stored on the second record as character variables and then converted to numerical data.

The third and final optional text record states the units used throughout the computations.

A.1.10 **Coordinate, Block, and Variable Identification.** The next segment of the file stores names for the coordinates, element blocks, material properties, and all variables stored in the file for identification on plots and printouts.

This segment also stores a print control table indicating which of the global, element, and nodal variables are printed out in each element block.

A.1.11 **Results.** The final segment of the file stores the values for all variables (Figure A.2). The variables are separated into two general classes: variables output at every timestep ("history" variables) and variables output at designated timesteps. This grouping allows an analyst to reduce the size of the output file. Variables output at designated timesteps are further subdivided into three classes: global, element, and nodal. Specifically,

- History
- Global
- Element
- Nodal.

} output at every time step (unless NVARGL is zero)

} output at designated timesteps.

Global variables refer to values of physical properties that apply to the large regions or the entire analysis, such as total energy or mass of the system. These properties can sometimes help indicate the accuracy of the analysis by checking whether energy or mass is conserved during the calculations.

Element variables refer to values of physical properties that apply to the finite element or the finite difference computational cell (grid block). Element variables are stored as a four dimensional array; hence, dynamic memory allocation is especially useful for reading element data.

Nodal variables refer to values of physical properties that apply to the computational FE or FD node.

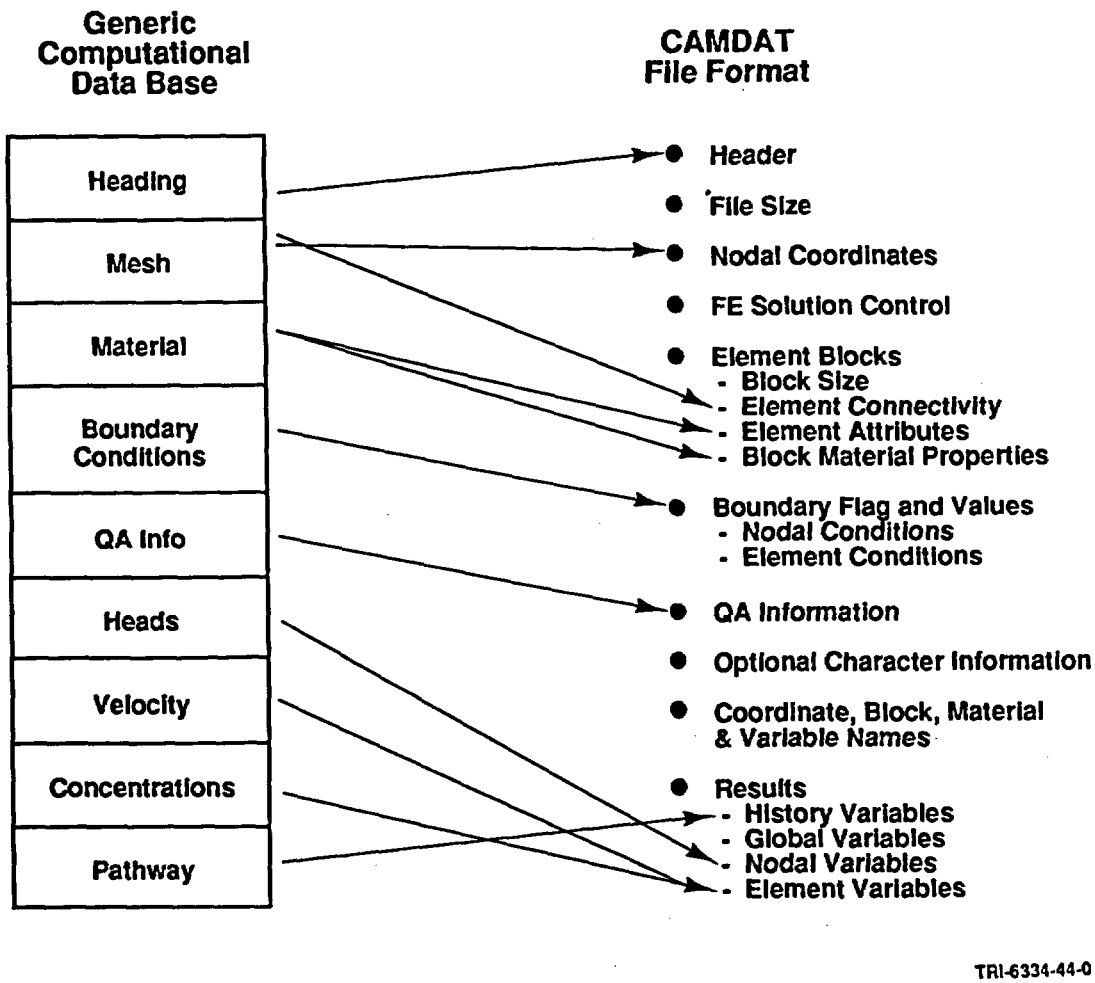


Figure A.2 Correspondence between generic computational data base and CAMDAT

A.2 File Format Specification

The computational data base file format is specified by the FORTRAN code fragment shown below (dimensioning statements and data transfer statements such as common blocks have been omitted). The appropriate section of the above text is referenced below for each record.

```
C=================================================================
C
C***Declarations*** (see Section A.1.1)
C
      PARAMETER NCDB=33
C                  ...omitted array dimensioning and data transfer
C                     statements
C
      OPEN (UNIT=NCDB,STATUS='OLD',ACCESS='SEQUENTIAL',FORM='UNFORMATED')
C
C***Read File Heading*** (see Section A.1.2)
C
      READ(NCDB) HEADER
C                  ...HEADER (CHARACTER*80)
C
C***Read Mesh Information*** (see Section A.1.3)
C
C...Read file sizing parameters
C
      READ(NCDB) NUMNOD,NDIM,NUMEL,NELBLK,NUMNPS,LNPSNL,NUMESS,
     &           LESSEL,LESSNL,LESSNL,NCDBVR
C                  ...Definition of mesh parameters
C                     NUMNOD - total number of nodes in the mesh
C                     NDIM   - number of dimensions
C                     NUMEL  - total number of elements
C                     NELBLK - number of element blocks
C                  ...Definitions for BC node and side sets
C                     NUMNPS - number of nodal point sets
                      LNPSNL - length of nodal point sets node list
                      NUMESS - number of element side sets
                      LESSEL - length of element side set element list
                      LESSNL - length of element side sets node list
C                  ...Data base version
                      NCDBVR - computational data base version number
C
C...Read nodal-point coordinates  (see Section A.1.4)
C
      READ(NCDB) ((COORD(I,J),I=1,NUMNOD),J=1,NDIM)
C
C...Read optimized element order map (see Section A.1.5)
C
      READ(NCDB) (MAP(I),I=1,NUMEL)
C                  ...use null read if not used
```

```
C
C...Read information for each element block (see Section A.1.6)
C
      DO 10 K=1,NELBLK
        READ(NCDB) IDEBLK,NUMELB,NELNOD,NATRIB,NUMPRP
C                 ...sizing parameters for block (see Section A.1.6.1)
C                    IDEBLK - unique integer ID for this block
C                    NUMELB - number of elements in this block
C                    NELNOD - number of nodes defining element
C                             connectivity
                     NATRIB - number of attributes for this element
                     NUMPRP - number of block material properties
C
        READ(NCDB) ((ICONN(J,I),J=1,NELNOD),I=1,NUMELB)
C                 ...connectivity for this block (see Section A.1.6.2)

        READ(NCDB) ((ATTRIB(J,I),J=1,NATRIB),I=1,NUMELB),
     &                (XMATPR(J),J=1,NUMPRP)
C                 ...ATTRIB - element block attributes (see Section
C                                                        A.1.6.3)
C                    XMATPR - block material properties
   10 CONTINUE
C
C***Read Boundary Condition Information*** (see Section A.1.7)
C
C...Read nodal point sets data (4 integer and 1 real data records)
C   (see Section A.1.7.1)
C
      READ(NCDB)(IDNPS(I),I=1,NUMNPS), (NAMNPS(I),I=1,NUMNPS)
C                 ...IDs for nodal point sets
C                    optional 8*CHARACTER names for nodal point sets
      READ(NCDB)(NPSTCT(I),I=1,NUMNPS)
C                 ...number of nodes in each nodal point set
      READ(NCDB)(IPTNPS(I),I=1,NUMNPS)
C                 ...pointers for locating each nodal set in node list
      READ(NCDB)(LSTNPS(I),I=1,LNPSNL)
C                 ...concatenated list of nodal point sets
      READ(NCDB)(FACNPS(I),I=1,LNPSNL)
C                 ...concatenated list of corresponding factors for
C                    nodal point sets
C
C...Read element side sets data (7 integer and 1 real data records)
C   (see Section A.1.7.2)
C
      READ(NCDB)(IDESS(I),I=1,NUMNPS),(NAMESS,I=1,NUMESS)
C                 ...IDs for each element side set
C                    optional 8*CHARACTER names for element side sets
      READ(NCDB)(NEESS(I),I=1,NUMESS)
C                 ...number of element sides in each element side set
      READ(NCDB)(NNESS(I),I=1,NUMESS)
C                 ...number of nodes associated with each element
C                    side set
```

```
      READ(NCDB)(IPEESS(I),I=1,NUMESS)
C                  ...pointers for locating each element side set in
C                     concatenated list of element sides
      READ(NCDB)(IPNESS(I),I=1,NUMESS)
C                  ...pointers for locating nodes in concatenated node
C                     list associated with each element side set
      READ(NCDB)(LTEESS(I),I=1,LESSEL)
C                  ...concatenated list of elements comprising side sets
      READ(NCDB)(LTNESS(I),I=1,LESSNL)
C                  ...concatenated list of nodal points associated with
C                     element side sets
      READ(NCDB)(FACESS(I),I=1,LESSNL)
C                  ...concatenated list of corresponding factors for
C                     nodes of the element side sets
C
C***Read Quality Assurance (QA) Information*** (see Section A.1.8)
C
      READ(NCDB) NQAREC
C                  ...read the number of QA records (≥ 1)
        DO 20 IQA=1,MAX(1,NQAREC)
          READ(NCDB) (QAINFO(I,IQA),I=1,4)
C                  ...I=1 code name (CHARACTER*8)
C                     I=2 code descriptor (CHARACTER*8)
C                     I=3 calculation date (CHARACTER*8)
C                     I=4 calculation time (CHARACTER*8)
   20   CONTINUE
C
C***Read Optional Text*** (see Section A.1.9)
C
      READ(NCDB) NXINFO
C                  ...read number of optional records
C
      DO 30 I = 1,NXINFO
        READ(NCDB) INFO(I)
C                  ...read any optional information (CHARACTER*80)
   30 CONTINUE
C
C***Read Variable Identification*** (see Section A.1.10)
C
C...Read the coordinate names
C
      READ(NCDB) (NAMECO(M),M=1,NDIM)
C                  ...NAMECO - coordinate names (CHARACTER*8)
C
C...Read element block, element attribute, and material property names
C
      READ(NCDB) (NAMELB(I),I=1,NELBLK),
     &        (NAMATR(I),I=1,NATRIB),
     &        (NMATPR(I),I=1,NUMPRP)
C                  ...NAMELB - element block names (CHARACTER*8)
C                     NAMATR - element attribute names(CHARACTER*8)
C                     NMATPR - material property names(CHARACTER*8)
```

```
C
C...Read history, global, nodal, and element variable names
C
      READ(NCDB) NVARHI,NVARGL,NVARND,NVAREL
C                  ...parameter definitions
C                     NVARHI - number of history variables
C                     NVARGL - number of global variables
C                     NVARND - number of nodal variables
C                     NVAREL - number of element variables
C
      READ(NCDB) (NAMHIV(I),I=1,NVARHI),
     &        (NAMGLV(I),I=1,NVARGL),
     &        (NAMNDV(I),I=1,NVARND),
     &        (NAMELV(I),I=1,NVAREL)
C                  ...read names of history, global, nodal,
                      and element variable names (CHARACTER*8)
C
C...Read array map of variables output to data base file
C
      READ(NCDB)((ISEVOK(I,J),I=1,NVAREL),J=1,NELBLK)
C                  ...ISEVOK(i,j) refers to element variable i of
C                     element block j; a value of 0 indicates
C                     data was NOT output (value≠0, otherwise)
C
C***Read Analysis Results*** (see Section A.1.11)
C
C...Read time step information and history flag
C
      DO 100 ITIME=1,NSTEP
C                  ...when reading the data base, value of NSTEP is not
C                     needed since an EOF marker can terminate reading
        READ(NCDB) TIME(ITIME), HIFLAG(ITIME)
C                  ...TIME must increase monotonically)
C                  ...HIFLAG (history flag) is 0.0 (real--avoids mixing
C                     variable types) when all variables were output,
C                     nonzero when only history variables output
C
C...Read history variables
        READ(NCDB) (VALHIV(IVAR),IVAR=1,NVARHI)
C
C...Read global variables
C
        IF (HIFLAG .EQ. 0.) THEN
C                  ...read other variables only if HIFLAG = 0.
          READ(NCDB) (VALGLV(IVAR),IVAR=1,NVARGL)
C
C...Read nodal value variables for current time step
C
          DO 70 IVAR = 1,NVARND
            READ(NCDB) (VALNDV(N,IVAR,ITIME),N=1,NUMNOD)
   70     CONTINUE
```

```
C
C...Read element variables for current time step
C
          DO 90 IBLK=1,NELBLK
            DO 80 IVAR=1,NVAREL
              IF (ISEVOK(IVAR,IBLK) .NE. 0) THEN
                READ(NCDB) (VALELV(IEL,IVAR,IBLK,ITIME),
     &                        IEL=1,NUMELB(IBLK))
C                  ...IEL is the element index in a block
              ENDIF
   80       CONTINUE
   90     CONTINUE
        ENDIF
  100 CONTINUE
C
      RETURN
      END
C
C-----------------------------------------------------------------------
```

A.3 Possible Changes in CAMDAT Data Base

Possible changes to the above file format include

- Relocating the coordinate names array to the above coordinate read statement
- Relocating the block names array to the above element block read statement
- Relocating the element attribute and material property names array to after the connectivity matrix read statement
- Relocating all file sizing integers to the beginning of the file
- Relocating the QA section to the beginning of the file.

Appendix B: Secondary Data Base

The purpose of Appendix B is to

- Generally describe the secondary data base
- Specify the file format using a FORTRAN code fragment.

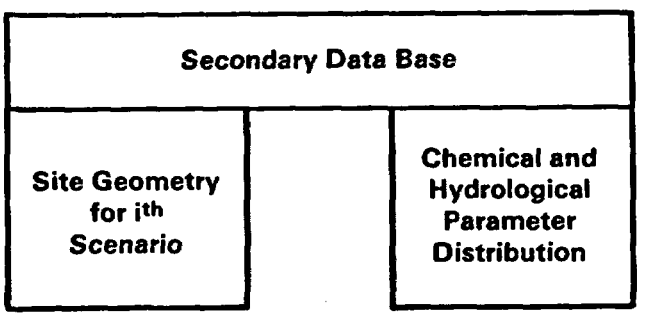
B.1 General Description of Secondary Data Base

The secondary data base stores the information that defines the conceptual model of the disposal system as it concerns a particular release scenario; in other words, each release scenario may have a secondary data base. Although text on the assumed important physical processes for the scenario are not stored, all other data necessary to model the disposal system for the release scenario are stored in the data base; for instance, data gaps existing in the primary data base will have been filled using objective interpolation or expert judgment.

Because the information will be updated as new data are entered into the primary data bases, potentially altering the conceptual model, the secondary data base possesses two general features:

- ASCII file format
- Two file purposes: storing model stratigraphy and storing parameter distributions (Figure B.1).

Unlike the computational data base, CAMDAT, data are stored in ASCII format, which makes entering and modifying data easier. Because the data will constantly change, several separate files are used to reduce the chance for random errors corrupting other sections of the data base.



TRI-6334-91-0

Figure B.1 The secondary data base consists of two separate file groups

B.2 Common Elements in File Formats

Information is stored in the secondary data base files so that the data are accessible by both a relational data base code and translators and support modules of the compliance assessment system. An example template of the storage scheme follows.

B.2.1 File Structure. All secondary data base files store information

- Sequentially
- In ASCII
- Readable with CAMCON's free-field or FORTRAN's list-directed read statements.

Thus, the file is readily read and used by relational data base codes (after removing the three file heading records).

In all files, the data fields are separated by commas for easy access by CAMCON's free-field reader (or FORTRAN's list-directed reader). The formats given for variables which follow are used only as guidance for data entry.

B.2.2 Header. For the compliance evaluation, the scenario identification for the conceptual model, model scale, and the type of file is recorded on the first record. For the final assessment of the WIPP, the secondary data base files will be identical for each scenario and model scale. The first record stores

1. IDSCNR - succinct scenario ID (ALL for final assessment) (CHARACTER*8)
2. SCLMOD - scale of conceptual model (CHARACTER*8); choices are REGIONAL, SOURCE, LOCAL, or ALL
3. FILTYP - type of file (CHARACTER*8); choices are WELL LOCation, WELL ELevation, or DISTRIBution
4. TITLE - descriptive but brief title for stored data (CHARACTER*56).

B.2.3 File Size and Version. The second record stores:

1. NENTRY - number of entries (I4)
2. NUMIDS - number of ID variables (I4)
3. NUMVAL - number of numerical values per record (I4)
4. NUMTXT - number of text strings per record (I4)
5. NSDBVR - version number of secondary data base (CHARACTER*8).

B.2.4 Variable Names. The final general heading of a secondary data base file stores the variable names:

1. NAMIDS - names for ID variables (CHARACTER*8)
2. NAMVAL - names of numerical values (CHARACTER*8)
3. NUMTXT - names of text variables (CHARACTER*8).

As seen above, the general scheme is to place variables needed for searching records at the begining of a record, then value(s) of interest, then elaborating text.

B.3 Storage of Conceptual Model Stratigraphy

For the WIPP, stratigraphic layer data from DOE, and from potash, oil, and gas wells were combined to form a secondary data base. From this data base, a conceptual (and mathematical) model of the stratigraphy is developed.

The stratigraphic data are stored in two separate file types: well locations and layer depths. The default unit numbers, NSDB, of the file storing well locations and layer depths are 21 and 22, respectively.

B.3.1 Well Locations. In addition to the three file header records, the file records storing well locations are organized as follows:

- Identifier for organizing data (e.g., sorting)
  1. IDWELL - standard well identification for WIPP (CHARACTER*8)
  2. IDALT - alternate identification used for well (CHARACTER*8)
- Stored information
  3. XUTM - x-coordinate of well in UTM system (m) (I8)
  4. YUTM - y-coordinate of well in UTM system (m) (I8)
  5. XSTPLN - x-coordinate in New Mexico State Plan Coordinate system (ft) (I8)
  6. YSTPLN - y-coordinate in New Mexico State Plan Coordinate system (ft) (I8)
  7. TOWNSHP - township location of well (I2)
  8. RANGE - range location of well (I2)
  9. SECTION - section location of well (I2)
  10. XREF - x-coordinate reference point for UTM System (m) (I8)
  11. YREF - y-coordinate reference point for UTM System (m) (I8)
  12. IDOTHR - other identification used for well (CHARACTER*24)
- QA information
  13. INFOSR - primary source of data (CHARACTER*32)
  14. CATALG - cataloger (name of person making entry) (CHARACTER*24)
  15. CHDATE - date of last change (CHARACTER*8).

B.3.2 Layer Depths. The record format for the depths of stratigraphic layers is as follows:

- Identifier for organizing data (e.g., sorting)
  1. IDMTRL - standard material ID (e.g., stratigraphic layer) (CHARACTER*8)
  2. IDWELL - standard well ID for WIPP (CHARACTER*8)
  3. IDPARM - standard ID for material parameter (CHARACTER*8)
- Stored information
  4. ELEVAT - depth (or elevation) of top surface of material (e.g., surface, Culebra, or Salado) (E14.7)
  5. DATUM - reference datum for depth (or elevation) (E14.7)
  6. UNITS - measurement units (CHARACTER*8)
- QA information
  7. INFOSR - primary source of data (CHARACTER*32)
  8. CATALG - cataloger (CHARACTER*24)
  9. CHDATE - date of last change (CHARACTER*8).

As for all secondary data base files, the data (e.g., layer ID) is separated by commas for easy access by CAMCON's free-field reader (or the FORTRAN list-directed reader); consequently, the formats given are used as only guidance for data entry.

B.4 Storage of Parameter Data

The parameter information was stored in one file type: parameter properties and distributions. The default unit number, NSDB, is 23. The fourth section of the file stores eleven pieces of data relevent to the parameter:

- Identifiers for organizing data (e.g., sorting)
  1. IDMTRL - ID for material (CHARACTER*8)
  2. IDWELL - ID for well (CHARACTER*8)
  3. IDPARM - ID for material parameter (CHARACTER*8)
- Stored information
  4. MEANVL - parameter value used when not sampling (e.g., mean, mode, or median of distribution) (E14.7)
  5. LOWRNG - lower limit of range (E14.7)
  6. HIRNGE - upper limit of range (E14.7)
  7. SCALE - scale factor for MEANVL, LOWRNG, and HIRNGE (e.g., thickness if property is transmissivity) (E14.7)

8. DISTYP - type of distribution (CHARACTER*24)

9. UNITS - measurement units (CHARACTER*8)

- QA information

10. INFOSR - primary data source (CHARACTER*32)

11. CATALG - cataloger (CHARACTER*24)

12. CHDATE - date of last change (CHARACTER*8).

B.5 Example File Format

A FORTRAN code fragment using list-directed read statements is shown below. (WIPP files used a free-field reader.) Dimensioning statements and data transfer statements have been omitted. To use this file format with any particular relational data base code may require removing the first three file heading records.

```
C-----------------------------------------------------------------------
C
C***Declarations*** (see sections B.2.1 and B.4)
C
      PARAMETER NSDB=23
C                  ...omitted array dimensioning and data transfer
C                     statements
C
      OPEN (UNIT=NSDB,STATUS='OLD',ACCESS='SEQUENTIAL',FORM='FORMATED')
C
C***Read File Heading***  (see section B.2.2)
C
      READ(NSDB,*) IDSCNR,SCLMOD,FILTYP,TITLE
C                  ...IDSCNR - succinct scenario ID (CHARACTER*8)
C                             'ALL' for final assessment
C                     SCLMOD - scale of model (CHARACTER*8)
C                             choices: REGIONAL, SOURCE, LOCAL, or ALL
C                     FILTYP - type of file (CHARACTER*8)
C                             choices: WELL_LOC, WELL_EL, or DISTRIBution
C                     TITLE  - title for stored data (CHARACTER*56)
C
C***Read File Size***  (see section B.2.3)
C
      READ(NSDB,*) NENTRY,NUMIDS,NUMVAL,NUMTXT,NSDBVR
C                  ...NENTRY - number of entries (I4)
C                     NUMIDS - number of ID variables (I4)
                      NUMVAL - number of numerical values (I4)
                      NUMTXT - number of text variables (I4)
C                     NSDBVR - version number of secondary data base (I4)
```

```
C
C***Read Parameter Distribution Names***  (see section B.2.4)
C
      READ(NSDB,*) (NAMIDS(I), I=1,NUMIDS)
                   (NAMVAL(J), J=1,NUMVAL)
                   (NUMTXT(K), K=1,NUMTXT)
C
C***Read Parameter Distributions***   (material properties and scenario
C                                      probabilities)  (see Section B.4.1)
C
      DO 10 I=1, NENTRY
        READ(NSDB,*) IDMTRL,IDWELL,IDPARM,MEANVL,LOWRNG,HIRNGE,SCALE,
    &                DISTYP,INFOSR,CATALG,CHDATE
C                 ...IDMTRL - ID for material (CHARACTER*8)
C                    IDWELL - ID for well (CHARACTER*8)
C                    IDPARM - ID for material parameter (CHARACTER*8)
C                    MEANVL - "average" value of parameter (E14.7)
C                    LOWRNG - lower limit of range (E14.7)
C                    HIRNGE - upper limit of range (E14.7)
C                    SCALE  - scale factor for MEANVL (E14.7)
C                    DISTYP - type of distribution (CHARACTER*24)
C                    INFOSR - primary data source (CHARACTER*32)
C                    CATALG - name of person making entry (CHARACTER*24)
C                    CHDATE - date of last change (CHARACTER*8)
  10  CONTINUE
C
C=================================================================
```

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