Study Plan for
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Three-Dimensional Rock Characteristics Models

U. S. Department of Energy
Office of Civilian Radioactive Waste Management
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Study 8.3.1.4.3.2 **Three-Dimensional Rock Characteristics Models**

Study Plan for the

Three-Dimensional Rock Characteristics Models Study

Site Characterization Plan
Study 8.3.1.4.3.2.

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YUCCA MOUNTAIN SITE CHARACTERIZATION PROJECT
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ABSTRACT

The Yucca Mountain site in southern Nevada has been identified as a potential location for a high-level nuclear waste repository. This Study Plan describes an integrative modeling activity, which will merge various types of measured or observed geologic, hydrologic, and engineering data, derived from a large number of site characterization studies, with other kinds of information and produce numerical models of selected material properties ("rock characteristics") in their proper spatial positions. These numerical models of material properties will be used by a group of analytical activities focused on evaluating the behavior of various engineered features, the effects of construction and operating practices, and the waste-isolation performance of the overall repository system, including the effects of the emplaced radioactive wastes. As such, the Study is anticipated to be one of the principal means of summarizing, integrating, and reconciling the diverse suite of earth-science data acquired through site characterization and of recasting that data in formats specifically designed for use in further modeling of the various (coupled) physical processes operating at the Yucca Mountain site.

Because the Study will produce numerical descriptive models of the Yucca Mountain site on an ad hoc basis to meet the input requirements of design-evaluation and performance-assessment analyses, and because much of the site-characterization information to be used in constructing these models has yet to be acquired, it is not possible to describe in detail the exact methodology(ies) and product(s) of this Study. This Study Plan, therefore, describes a relatively comprehensive "toolbox" of techniques that could be used to produce the required numerical models of rock characteristics. These techniques may be divided into two principal categories: methods for modeling the geometric-framework of arbitrary rock units and methods for assigning specific material-properties values to locations within those units.

Geometric modeling methods may be further subdivided into *surface-oriented* and *volume-oriented* techniques. Each technique offers certain advantages and possesses certain limitations in the context of the Yucca Mountain site. Methods for assigning the appropriate material-properties in-fill of a rock properties model may be classified as *estimation* or *simulation* techniques. Estimation attempts to assign the most accurate value possible (using the selected algorithm) to each spatial location within a model. Simulation, on the other hand, attempts to assign values that are statistically "likely" in terms of the *overall model* or geologic context, but without those values necessarily being the most-likely value at any specific location within that model. Simulation is generally associated with quantitative, Monte-Carlo-style efforts to assess geologic uncertainty. Both estimation and simulation techniques may produce models that are or are not spatially variable, depending upon the intended use of the specific model. Variable-property models may or may not attempt to respect quantitative patterns of spatial continuity (spatial correlation) that could be present in the natural environment; those approaches that incorporate spatial continuity patterns are broadly grouped as *geostatistical* techniques.

Section 1 describes the purpose and objectives of this Study and the technical issues addressed as part of the Study. Section 2 provides a description of the actual technical activities and how these activities will be accomplished. Section 2 also contains a discussion of the anticipated direction of modeling activities under this Study, which is based upon preliminary rock-characteristics modeling conducted prior to preparation of this Study Plan. A description is provided of the relationship between this modeling Study and activities classified both as providing

data and as evaluating the resulting models. The relationship of this Study to other, similar types of integrative-modeling activities is also described. Section 3 summarizes how the resulting models of material properties will be applied in the resolution of specific design and performance-assessment issues described in the Yucca Mountain Site Characterization Plan. Finally, Section 4 presents high-level schedules and associated milestones related to site suitability and potential licensing of a repository at Yucca Mountain.

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1.0 PURPOSE AND SCOPE OF THE STUDY

The U.S. Department of Energy is conducting studies of a potential site at Yucca Mountain, Nevada, which has been proposed as the location for a high-level nuclear waste repository. Geologic, hydrologic, and geotechnical information about the site will be required for both engineering design studies and for activities directed toward assessing the waste-isolation performance of the overall repository system. Acquisition and evaluation of this basic geologic information is the focus of a multidisciplinary site-characterization effort being conducted on behalf of the Department of Energy by several federal agencies and other organizations as part of the Yucca Mountain Site Characterization Project. Figure 1.1 shows the location of the general Yucca Mountain area in southern Nevada. The location of the proposed underground facilities, also shown on Figure 1.1, represents preliminary design concepts developed prior to detailed site characterization.

The Yucca Mountain site consists of a gently eastward-dipping sequence of volcanic tuffs, principally welded ash flows, with intercalated nonwelded and reworked units. Various types of alteration phenomena, including devitrification, zeolitization, and the formation of clays, have been superimposed upon the primary lithologies. The units are variably fractured, and faulting has offset the various units, locally juxtaposing markedly different lithologies. A comparison of differing stratigraphic terms that have been used to describe the rocks at Yucca Mountain is shown in Figure 1.2.[1] The potential repository would be excavated in the central portion of the Topopah Spring Tuff of the Paintbrush Group, within the TSw2 unit defined by Ortiz and others (1984). Accordingly, most design interest is focused on the Topopah Spring Tuff and immediately adjacent units. By comparison, performance assessment (PA) focuses on evaluating the waste-isolation behavior of the entire repository system within a much-larger geologic volume comprising much of the stratigraphic section underlying Yucca Mountain. Compliance with regulations concerned with waste isolation generally must be demonstrated at what is termed the *accessible environment* in 10 CFR 60.2, or outer limit of the controlled area (Figure 1.1).

1.1 Objectives of the Study

The Three-Dimensional Rock Characteristics Models Study, Study 8.3.1.4.3.2, is one of a number of formal "studies" and other activities described in the Yucca Mountain Site Characterization Plan (DOE, 1988; hereinafter referred to simply as the Site Characterization Plan or SCP) that are involved in three-dimensional modeling (broadly defined) of the potential repository site. The principal purpose of this study (Study 8.3.1.4.3.2) is to synthesize various types of site characterization information produced by many different SCP studies and to produce numerical models (plural intended) of geology and material properties ("rock characteristics") specifically for use in engineering-design analyses and performance-assessment calculations. These further analyses are required to model the physical-process behavior of different natural systems, either as they exist in their natural state or as they may be affected by the presence of the potential repository and contained heat-producing nuclear waste. Although other types of synthetic modeling,

1. Until recently revised formally by Sawyer and others (1994), stratigraphic nomenclature at Yucca Mountain made reference to the Paintbrush *Tuff*, which was comprised of the Tiva Canyon, Yucca Mountain, Pah Canyon, and Topopah Spring *Members*. References to older literature should be evaluated with this change in terminology in mind.

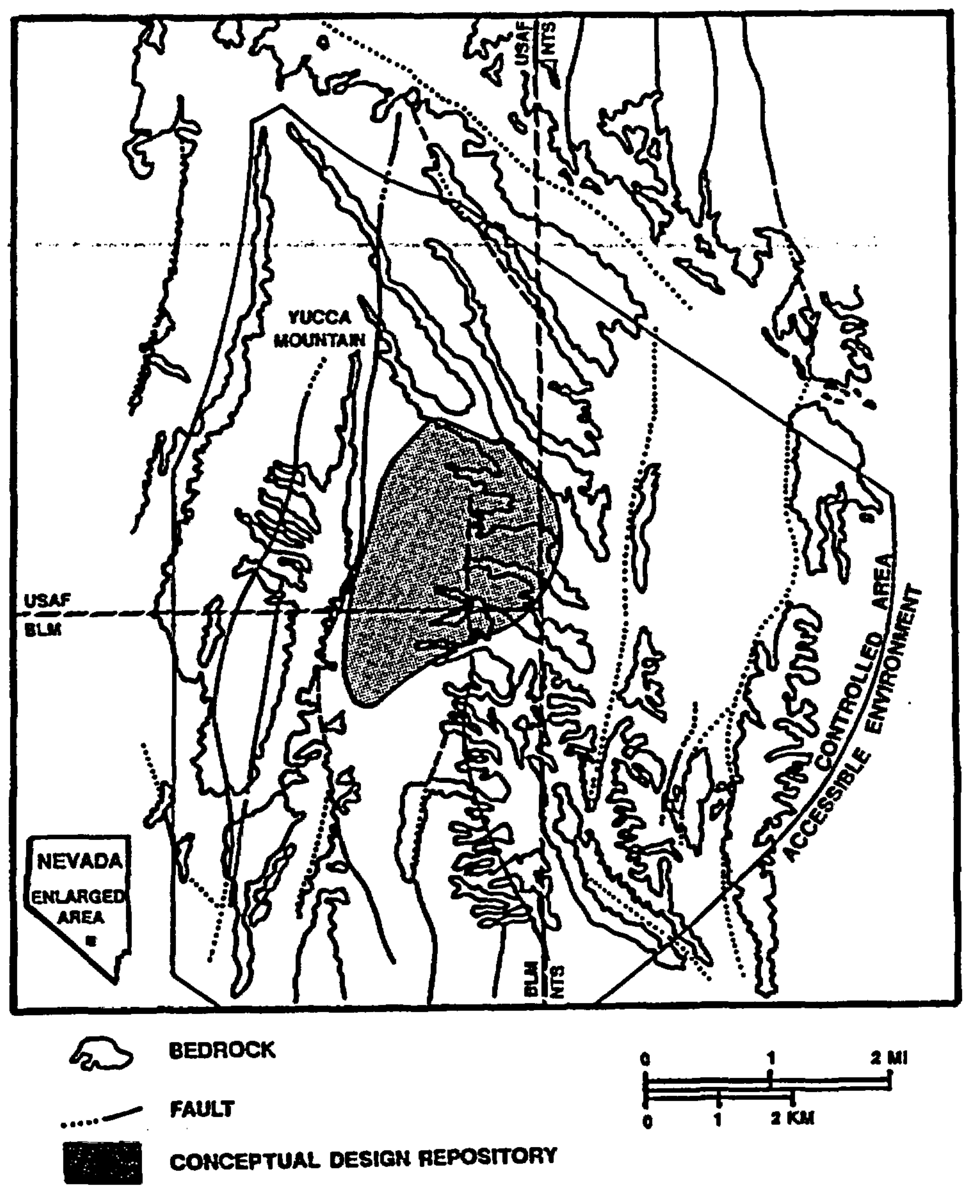

Figure 1.1 Index map showing the location of the potential Yucca Mountain repository site in southern Nevada

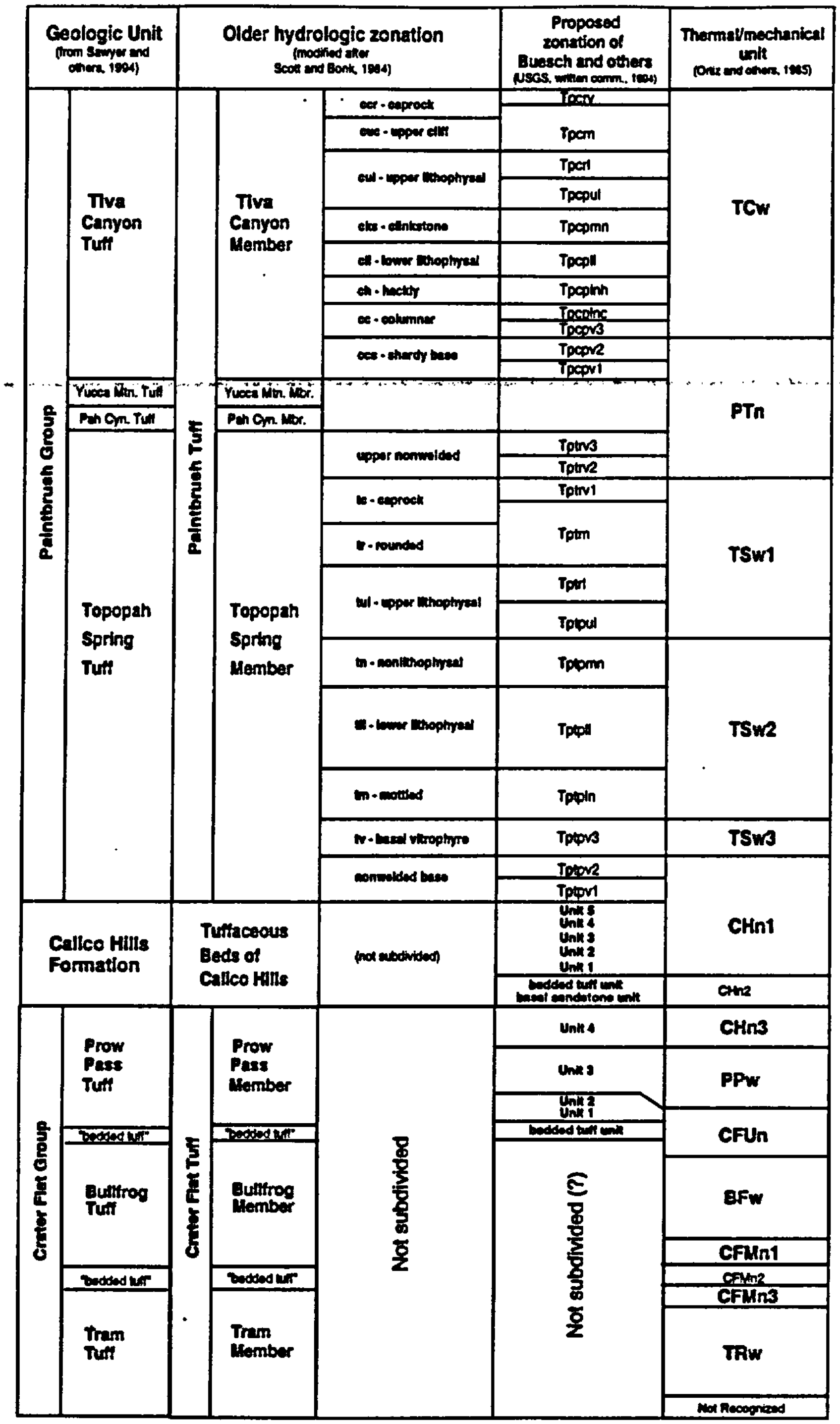

Figure 1.2 Comparative stratigraphic terminology in common usage at Yucca Mountain. Sequential codes used in proposed nomenclature of D.C. Buesch (USGS, written communication, 1994): Tpc - Tertiary Tiva Canyon Tuff of the Paintbrush Group, Tpt - Tertiary Topopah Spring Tuff of the Paintbrush Group; c - crystal-rich, p - crystal-poor; u - upper, m- middle, l - lower; v - vitric, n - nonlithophysal, l - lithophysal; 1, 2, 3 - additional subdivisions from bottom to top).

including geologic framework modeling and modeling of material properties, will be conducted by other participants of the Yucca Mountain Project (as discussed throughout this Study Plan), the Three-Dimensional Rock Characteristics Models Study is anticipated to have a particularly close and direct tie to many performance modeling activities used in licensing arguments.

The objective of any particular modeling exercise under this Study will be to produce a numerical representation of the material properties important to a particular engineering-design or performance-assessment analysis, which spatially and statistically resembles the actual geology as closely as possible. This numerical representation must also be created in a format and conceptual framework that is defined by the specific requirements of the analysis. Simplifications of the complex system must capture the computationally significant features, while at the same time allowing the process-modeling solution to be computationally tractable.

Although it is evident that all modeling of the Yucca Mountain site must respect the underlying common entity that is Yucca Mountain, and thereby exhibit certain features in common, the fact that different Project-level modeling activities are unique and oriented toward the analysis of specific physical phenomena poses significant challenges for an integrative study such as this. Thus, explicit definition of an all-encompassing "three-dimensional rock characteristics model" (singular) and procedural details of a specific modeling process cannot be given in this Study Plan. Rather, the focus of this document is on the description of several different modeling approaches, any of which might be employed to create a model of rock characteristics suitable for further evaluation. Exhaustive, theoretical descriptions are not provided. Instead, a general description of each methodology is given and accompanied by a brief discussion of its suitability or limitations. A summary discussion, Section 2.3, *Anticipated Direction of Modeling Activities*, is provided based upon existing, limited, scoping-type studies and an understanding of the licensing process as described in the Yucca Mountain Site Characterization Plan. Although the specific material properties to be modeled depend upon the ultimate use of the rock characteristics model(s) produced, it is virtually certain that spatial models of a limited suite of "framework" hydrologic properties (e.g., porosity, hydraulic conductivity), thermal and mechanical properties (porosity, bulk density, thermal conductivity, compressive strength), and certain geochemical or compositional properties (mineral abundances) will be generated by this Study.

1.2 Technical Issues Addressed

The models generated by the Three-Dimensional Rock Characteristics Models Study will be used throughout the Yucca Mountain Project to address a number of technical issues related to the licensing of a potential repository. A listing of some of these issues is presented in Table 1.1. At a subsidiary level, the majority of these referenced issues have stated "Information Needs" that read "Site information needed for _____." Although site information *per se* is what is specified as required for resolution of the technical issues, interpretive reading of these Information Needs indicates that what is really required is generally some type of comprehensive model of the site. Generally speaking, the Issues in Table 1.1 cannot be resolved simply on the basis of isolated measurements or observations. It is the integration of many types of site characterization information from numerous studies into a coherent representation of the geologic setting of Yucca Mountain that provides a basis for issue resolution. Several technical issues listed in the SCP have no stated information need that explicitly calls for "site information," yet it is clear from the context that site information is required at some level (see also Appendix IV to 10 CRF 960). These issues have also been included in Table 1.1, together with a brief notation as to why such inclusion is justified in terms of this study. A more detailed listing of the Information Needs addressed by this Study is given in Tables 3.1 and 3.2.

Table 1.1 Technical Issues Addressed Through Models Created by the Three-Dimensional Rock Characteristics Models Study (taken from the SCP), with Notes on Related Needs for Site-Specific Information and Models Relevant to this Study

Issue 1.1	Will the mined geologic disposal system meet the system performance objectives for limiting radionuclide releases to the accessible environment as required by 10 CFR 60.112 and 40 CFR 191.13?
Information Need 1.1.1	Site information needed to calculate releases to the accessible environment.
Issue 1.2	Will the mined geologic disposal system meet the requirements for limiting individual doses in the accessible environment as required by 40 CFR 191.15?
	Doses are related to the radionuclide releases of Issue 1.1
Issue 1.6	Will the site meet the performance objective for pre-waste emplacement ground-water travel time as required by 10 CFR 60.113?
Information Need 1.6.1	Site information and design concepts needed to identify the fastest path of likely radionuclide travel and to calculate the ground-water travel time along that path.
Issue 1.8	Can the demonstrations for favorable and potentially adverse conditions be made as required by 10 CFR 60.122?
	The conditions enumerated in 10 CFR 60.122 are clearly tied to descriptive site information and models based on that information.
Issue 1.11	Have the characteristics and configurations for the repository and repository engineered barriers been adequately established to (a) show compliance with the post-closure design criteria of 10 CFR 60.133, and (b) provide information for the resolution of the performance issues?
Information Need 1.11.1	Site characterization information needed for design.
Issue 1.12	Have the characteristics and configurations of the shaft and borehole seals been adequately established to (a) show compliance with the post-closure design criteria of 10 CFR 60.134, and (b) provide information for the resolution of the performance issues?
Information Need 1.12.1	Site, waste package, and underground facility information needed for design of seals and their placement methods.
Issue 2.4	Can the repository be designed, constructed, operated, closed, and decommissioned so that the option of waste retrieval will be preserved as required by 10 CFR 60.111?
Information Need 2.4.1	Site and design data required to support retrieval.
Issue 2.7	Have the characteristics and configurations of the repository been adequately established to (a) show compliance with the preclosure design criteria of 10 CFR 60.130 through 60.133 and (b) provide information for the resolution of the performance issues?
	Determination of the "characteristics and configurations of the repository" require site information in a manner similar to Issue 2.4.

Table 1.1 Technical Issues Addressed Through Models Created by the Three-Dimensional Rock Characteristics Models Study (taken from the SCP), with Notes on Related Needs for Site-Specific Information and Models Relevant to this Study

Issue 4.2	Are the repository design and operating procedures developed to ensure nonradiological health and safety of workers adequately established for the resolution of the performance issues?
Information Need 4.2.1	Site and performance assessment information needed for design.
Issue 4.4	Are the technologies of repository construction, operation, closure, and decommissioning adequately established to support resolution of the performance issues?
Information Need 4.4.1	Site and performance assessment information needed for design.

2.0 SCOPE OF WORK

The program of work described in the Site Characterization Plan describes a systematic, detailed program of site characterization and analysis directed toward preparation of required licensing documents. Prior to the site characterization program, investigations of the Yucca Mountain site focused on determining the ability of the site to meet various siting guidelines specified in both Department of Energy and Nuclear Regulatory Commission regulations (10 CFR 960 and 10 CFR 60, respectively). This Study proposes to develop numerical models of geology, derived from all available data, using the most appropriate geometric, statistical, and geostatistical techniques to describe spatially variable rock-properties distributions. The Study is closely linked logically to two specific groups of studies. These are: (1) the studies in Investigation 8.3.1.4.2, "Geologic Framework of the Yucca Mountain Site" (an "investigation" is the next-higher level grouping of work described in the SCP above a "study), and (2) Study 8.3.1.4.3.1, the Systematic Acquisition of Site-Specific Subsurface Information Study, which forms part of Investigation 8.3.1.4.3, "Development of Three-Dimensional Models of Rock Characteristics at the Repository Site" that also includes the current Study. However, the modeling conducted under the Three-Dimensional Rock Characteristics Models Study transcends these associations. This Study is a synthetic modeling activity strategically placed between site characterization and design-evaluation and performance-assessment analyses.

2.1 Data

Because the Three-Dimensional Rock Characteristics Models Study is a synthetic study integrating a wide variety of site-characterization information, it is difficult to enumerate all of the various data that will be incorporated into the resulting models. Essentially, any and all types of descriptive information on "rock characteristics" obtained from the Yucca Mountain site may be utilized, together with other, non-site information such as general geologic concepts related to the regional geologic setting or fundamental behavior of rock masses. The primary determinant of the data required for the Study is the ultimate use of the rock characteristics model(s) produced using that data. However, it is virtually certain that spatial models of hydrologic properties (e.g., porosity, hydraulic conductivity), thermal and mechanical properties (porosity, bulk density, thermal conductivity, compressive strength), and certain geochemical or compositional properties (zeolite abundances, proportions of silica polymorphs) will be generated by this Study to meet the requirements of the end-user performance assessment and design activities (see also discussion of how this Study relates to other SCP studies and activities in section 2.4).

2.1.1 Surface Geologic Mapping

Three-dimensional models are required because the geologic environment of Yucca Mountain is a three-dimensional solid. Thus, a major requirement is to obtain information that is distributed throughout that three-dimensional volume. Surface mapping, conducted largely under Studies 8.3.1.4.2.1 ("Characterization of Vertical and Lateral Distribution of Stratigraphic Units within the Site Area") and 8.3.1.4.2.2 ("Characterization of the Structural Features within the Site Area"), will provide a rather comprehensive suite of data regarding the distribution of different rock types and their material properties on the present-day topographic surface. Surface descriptions include not only information derived from maps *per se*, but also descriptions obtained from outcrop transects and stratigraphic profiles. This information will be incorporated, as appropriate, by mapping the relevant geologic attributes into their proper spatial position within the model coordinate system through digitizing or other methods.

2.1.2 Subsurface Geologic Data

Subsurface data from logging and description of surface-based drill holes will form a major portion of the information on which the three-dimensional rock characteristics models will be based. Again, the proper location of various geologic features observed in boreholes, such as contacts between geologic units and structural breaks (faults, joint sets) will be mapped directly into the appropriate coordinate system to constrain the modeling of unsampled and unobserved volumes. Another significant, although stratigraphically limited, source of subsurface information will be that obtained in the various underground workings or (relatively short) drill holes constructed as part of the Exploratory Studies Facility (and presumably later from the potential repository itself during performance-confirmation studies). The means of incorporating this information is similar to that for drill hole information. Surveyed coordinates of the ESF workings and test alcoves are also required. A non-exhaustive list of some typical information obtained through geologic logging of drill core or underground mapping is presented in Table 1.1

Table 1.1 Rock Characteristics Information Typically Obtained Through Geologic Mapping or Logging of Drill Core

Category of Information	Specific Attributes	Principal Sources of Data (SCP Studies)
Geologic Units	depth, elevation, attitude, areal extent	8.3.1.4.2.1; 8.3.1.4.2.3; 8.3.1.4.3.1
Thermal/Mechanical Units (or other relevant stratigraphic subdivisions)	depth, elevation, attitude, areal extent	8.3.1.4.2.1; 8.3.1.4.2.3; 8.3.1.4.3.1
Lithologic Descriptions	degree of welding, abundance of pumice, lithic clasts, and lithophysae; types and intensity of alteration	8.3.1.3.2.1; 8.3.1.3.2.2; 8.3.1.4.2.1; 8.3.1.4.3.1; 8.3.1.14.2.1
Fault Zones	location, approximate orientation, internal character, displacement	8.3.1.4.2.2; 8.3.1.4.2.3; 8.3.1.4.3.1
Fractures	location, frequency, approximate orientation and aperture, mineralization	8.3.1.3.2.1; 8.3.1.4.2.2; 8.3.1.4.3.1 8.3.1.14.2
Core Recovery Information	absolute quantity and percent core recovered	8.3.1.4.2.1; 8.3.1.4.3.1; 8.3.1.14.2.1
Rock Integrity Information	RQD	8.3.1.4.3.1; 8.3.1.14.2.1

2.1.3 Laboratory Measurements of Material Properties

Quantitative values for rock material properties of interest are necessary as well as the more geometric "framework" information described thus far. These data form the basis for the ultimate purpose of the study: the creation of numerical "rock characteristics models." Although the specific material properties to be incorporated in any specific rock characteristics model will be determined by the purpose of the subsequent process-modeling activity, it is possible to make some generalization regarding the sources and types of material-properties data that will be required. A brief listing of important classes or types of laboratory material properties identified in the SCP is presented in Table 2.2. A more comprehensive listing of properties is given in Table 2.6, in the section discussing specific data-providing studies.

Table 2.2 Classes of Material Properties to be Modeled by the Three-Dimensional Rock Characteristics Study

Classes of Material Properties	Examples	Principal Sources of Data (SCP Studies)
Hydrologic Properties	porosity, water content, saturation, matrix permeability, matric potential, moisture-retention characteristics, sorptivity	8.3.1.2.2.3; 8.3.1.4.3.1
Thermal Properties	heat capacity, thermal conductivity, coefficient of thermal expansion	8.3.1.15.1.1; 8.3.1.15.1.2
Mechanical Properties	compressive strength, Poisson's ratio, Young's modulus	8.3.1.15.1.3; 8.3.1.15.1.4
Compositional Properties	mineralogy, percent composition	8.3.1.3.2.1; 8.3.1.4.2.1

Rock samples for laboratory testing of material properties may be obtained from outcrops, from drill core (and possibly cuttings), and from the underground workings or drill holes within the Exploratory Studies Facility. In addition to the quantitative measurements of material properties, other information will be required to incorporate these data into a comprehensive model. This supporting information includes: spatial location of samples; rock-unit assignments of samples; location relative to faults, stratigraphic contacts, or other features important to spatial variability; and assurance that the type of property represented is compatible with other measurements of the "same" property (for example, there are several techniques for measuring porosity; these may not be equivalent for some purposes; compare Bush and Jenkins [1970] and Soeder *et al.* [1991] with Boyd *et al.* [1994]). The appropriate numerical values will be mapped into their proper spatial position within the coordinate system of the model.

2.1.4 Design- and Analysis-Related Input

Another type of data that is required for the three-dimensional models of rock characteristics created under this Study is design-related or analysis-related information. The analyses that are undertaken, for which these numerical models of rock properties serve as input, are undertaken for a particular purpose. As such, there are likely to be very specific requirements imposed on this modeling activity, such as the grid size for finite-element modeling, locations and orientations of grid blocks, and specific properties to be modeled. It is unlikely that a rock-properties model suitable for evaluation of total-system radionuclide releases will also be suitable for evaluation of stresses induced in a drift by thermal loading from spent nuclear fuel. The extent of the modeled volume, the required spatial resolution, and the material properties of interest (and modeling focus) are obvious constraints that derive directly from the ultimate users of these models. Depending upon the analysis, other design-related input, such as the location and dimensions of (actual or proposed) engineered features (drifts, ramps, test alcoves, etc.) may be required.

2.1.5 Other Relevant Site Data

In addition to the specific types of site data described in sections 2.1.1 through 2.1.4, there will be a variety of other types of site information that may prove useful for constructing three-dimensional models of rock characteristics in certain situations. Because most of the material-properties models produced by this Study are custom-built to meet a particular analytical need, it is difficult to describe these data and their use in detail. Nevertheless, various types of geophysical measurements (e.g., from seismic, magnetic, and electrical surveys conducted under Study 8.3.1.4.2.1) and remote-sensing surveys provide information regarding the character and spatial arrangement of subsurface materials. Non-laboratory tests of several types may provide useful information regarding rock properties, particularly on a scale larger than that for which measurement is possible in the laboratory (see also the discussion of scaling in section 2.2.2.4). Examples of these field tests are borehole measurements of vadose-zone air permeability or pump tests in the saturated zone.

Depending upon the type of "other relevant site data" and the purpose of the intended modeling exercise, it is possible that such data may be incorporated directly into the modeling effort, just as geologic data or a laboratory rock-property value would be used. Incorporation of large-scale measurements (e.g., borehole tests) as actual hard data used in the model construction is the easiest to accomplish. Other types of data, generally those which do not have a unique material-properties interpretation (for example, results of certain geophysical surveys), may more realistically be incorporated as soft data (such as discussed on page 19) and used to *constrain* a rock-properties model but not to control it. An alternative approach for sufficiently soft data might be to reserve them for use as part of model validation efforts, as discussed in a somewhat different context in section 2.5.2 through 2.5.4. Although that discussion focuses on comparison with "alternative" models, any model created by this study could be evaluated (and thus "incorporate" the data to some extent) by reference to the geophysical or pump-test signature implied by its distribution of rock properties. Methods for incorporating soft data in this sense of validation during model creation (as opposed to simple after-the-fact geophysical or hydrologic modeling of an extant properties model) are only poorly developed at present, but form an active area of research.

2.2 Methods

The specific methods to be employed in the construction of any particular three-dimensional rock characteristics model can only be determined when the criteria for a specific modeling activity are established. Modeling under this Study is not an end in itself. Inevitably, the overall focus is on *evaluating the consequences of a particular distribution of rock properties as they affect the operation of some physical process*, such as ground water flow and transport or thermal expansion of a rock mass. Because the consequences of these rock properties models affect the suitability of the Yucca Mountain site in terms of licensing criteria, there will also be a significant need to quantify the uncertainty in the models of material properties and to propagate that uncertainty through the physical process model(s) to quantify uncertainty in site performance.

Although the details of specific rock characteristics models cannot be defined *a priori*, there are two major aspects of the modeling that will be conducted under this Study which can be described in this Study Plan. These are techniques for modeling geometry and for modeling the spatial distribution of material properties within that geometry. Collectively, these modeling approaches comprise a toolbox of techniques from which can be selected the tools to deal with virtually any required model of the site.

2.2.1 Geometric-Framework Modeling

Modeling geometry generally is dependent upon the subdivision of the rocks forming a site into some set of coherent, internally similar stratigraphic units. It is also possible to create "geometric" distributions of material properties without reference to stratigraphic units of any sort (for example, Rautman and Flint, 1992).

The classical application of geometric modeling focuses on geologic, or more-or-less genetic, stratigraphic subdivisions of the rock sequence. Other applications may focus on stratigraphic subdivisions that aggregate materials with similar hydrologic or thermal/mechanical properties (e.g., Ortiz *et al.*, 1985). The type of stratigraphic subdivision utilized will depend upon the purpose of the modeling (and subsequent analytical) exercise. A principal requirement is that the data obtained by site characterization activities be flexible enough that the modeler may recast the rock sequence in whatever manner is required. For example, the major ash-flow sequences present at Yucca Mountain (Figure 1.2) consist of a welded core surrounded by poorly welded to nonwelded material, all of which was deposited essentially simultaneously. These major flow sequences are typically separated from one another by additional nonwelded, small-volume ash flow tuffs, ash-fall tuffs, and reworked tuffaceous deposits. For some analyses, the appropriate stratigraphic subdivision may focus on the distinction between welded and nonwelded lithologic types (e.g., the thermal/mechanical classification of Figure 1.2). In other modeling efforts, the proper focus may be on the entire genetic package from nonwelded base to nonwelded top (formal geologic nomenclature in Figure 1.2).

Geometric modeling in its simplest form merely consists of mapping actual observations of contacts between the selected stratigraphic subdivisions into their proper location within the model space. These (generally) scattered observations are then connected by some mechanism to form a coherent interpretive representation of the real world. The mechanisms by which the model is filled-in vary greatly in sophistication. Cross-sectional views of a model may be constructed simply by laying a straightedge between a contact observed at two different locations. Alternatively, considerable geologic intuition may go into the construction of a particular contact in zones of poorly known faulting or stratigraphic variability.

Manual methods of model construction involve the development of cross sections, long sections (parallel and perpendicular to structural dip, respectively), and level plans. Keeping the various views of a three-dimensional solid consistent in different orientations may be quite a challenge. Other manual methods of creating and viewing (implied) three-dimensional models of geometry may involve structure contour maps or other types of isopleth maps.

Computer-based geometric modeling techniques can result in essentially identical "views" of a model (i.e., cross section, long sections, and level plans). However, the bookkeeping involved in maintaining geometric consistency is typically handled through the implementation of the particular modeling package (computer-software considerations are discussed in Section 2.3.2). Two principal types of computerized modeling packages are available: surface-oriented and volume-oriented. These two types represent the algorithm(s) used to connect the scattered observations of unit contacts.

A surface-oriented algorithm essentially takes the observed contact locations and fits some type of (more-or-less smoothly) varying surface through those contact points. Once the surfaces have been created, regions within the model are either above or below a particular surface. Stratigraphic units may be defined by an upper bounding surface and a lower bounding surface. However, generally there is no "association" of an arbitrary point with a particular three-dimensional geologic unit (i.e., a volume), *per se*.

Faulting poses significant difficulties for most surface-oriented algorithms. Because the bounding surfaces are represented by mathematical expressions fitted to a collection of points, it is necessary that the described surface be mathematically continuous (in terms of computing a derivative). Since faults are, by definition, a specific type of discontinuity, some type of work-around is required. One such resolution is to fit surfaces to only the contact locations contained within a single fault block and the resulting surface is then truncated at the boundaries of that block. Other blocks are modeled in a similar manner, resulting in a collection of several different surfaces, each restricted to a finite, though irregular, x-y domain. The technique is limited, however, by data availability. In general, three points are required to define a plane. Thus, unless a minimum of three drill hole intercepts for a given contact are available within each fault block (rarely the case at Yucca Mountain), the approach may not be feasible without the creation of "pseudo-drill holes" by some (presumably subjective) method. An alternative resolution is to remove the effect of faulting by adding or subtracting the appropriate fault offset from the observed elevation of each contact with respect to some assumed reference block. The continuous mathematical surface is then fitted to the "prefaulted" set of contacts, and then offset in a manner indicated by the previously "undone" faulting. Ortiz *et al.* (1985) applied this method to the offset of thermal/mechanical contacts at Yucca Mountain with some success. The technique is wholly dependent upon being able to define a suitable "reference" block and being able to determine the amount of fault offset at each location relative to that reference. As the degree of structural complexity increases, this determination becomes problematical; generally, fault offsets are determined by examining the model and not vice versa. Thus, typically one ends up in the mutually contradictory positions of needing the offsets to define the surface and of needing the final position of the surface to define the offsets. Generally, surface modeling has been more effective in structurally uncomplicated projects exactly for these reasons.

In contrast to surface-oriented techniques, volume-oriented methods define three-dimensional solid volumes to represent stratigraphic units. The association of points within the volume with the nature of the volume itself is generally explicit. Creation of a volume-oriented model may be more time- and labor-intensive than the creation of an equivalent surface-oriented model because of the need to associate all positions in space with a particular unit designation. The method of volume creation may be relatively automatic through operation of some (generally black-box) algorithm, or it may rely partially on interpretive construction by an experienced geologist with only partial automation. The trade-off is between ease and rapidity of model creation and update versus the ability to induce subtle geologic complexity based largely on soft, qualitative information. Modeling using volume-oriented packages is hampered by faulting and other data deficiencies in a somewhat analogous manner as with surface-modeling packages. Automated volume-generation routines are particularly subject to generating geologically unreasonable models unless geologic interpretation is imposed through the specification of more-or-less arbitrary control points or the use of subjective "surface-editing" techniques. Functionally, all modeling techniques are subjective and represent interpretations of sparse, usually poorly distributed spatial data.

2.2.2 Material-Properties Modeling

The material-properties modeling aspect of three-dimensional rock characteristics modeling is focused on assigning geologically reasonable values for rock properties of interest at unsampled locations. There are a large number of potential techniques, each of which may be appropriate for certain classes of analytical problems. These techniques may be classified into two broad categories: estimation and simulation.

Estimation attempts to assign a "best-estimate" value to unsampled locations, where "best" is in the mind of the modeler. The estimated values may or may not be spatially variable, depending upon the purpose of the analysis. Simulation, on the other hand, attempts to assign values such that the statistical properties of the resultant model *as a whole* tend to reproduce some desired characteristics, without particular regard for the "accuracy" of the value at any individual location. Simulated models are generally used as input to some type of Monte-Carlo-style assessment of uncertainty.

Numerical modeling of material properties can be done manually, or with only very limited computational assistance (see, for example, the representative-value or nearest-neighbor approaches described in Section 2.2.2.1). More generally, however, the need to integrate a moderately large number of sample measurements, or to reproduce selected statistical characteristics of a sample population moves material-properties modeling beyond the realm of manual calculations. The numerical algorithms described in this section, both for estimating and for simulating the value of a material property at unsampled locations are all published and moderately well-established methods, and the majority of the techniques have been implemented in a number of different computer codes. Further discussion of specific computer programs and software packages is provided in section 2.3.2, "Computer Software Considerations."

2.2.2.1 Estimation

Representative-Value Approach

One of the most common and simplest methods of estimating the value of a material property at an unsampled location is the assignment of a "representative value." The specific value(s) selected as "representative" typically have a statistical basis derived from analysis of samples from within the area or volume to be estimated. An example might be to designate the mean (or median) value and to assign this single property to an entire volume of material judged to be sufficiently similar. Alternatively, the representative value may be determined on the basis of professional judgement based upon analogue sites elsewhere or by modifying some statistical analysis of local samples to account for general geologic knowledge.

The representative value approach has been widely used in hydrologic studies (Anderson and Woessner, 1992). For example, hydrogeologic units, such as aquifers and confining beds, may be defined and each assigned a single-valued set of material properties (e.g., porosity, hydraulic conductivity, storativity, etc.). In a regional-scale study, a single hydrogeologic unit may comprise several geologic formations that are judged sufficiently similar to one another. An example is the so-called Tertiary volcanic aquifer at Yucca Mountain, which aggregates essentially all the welded and nonwelded tuffs at the site into one "unit." For more detailed investigations, a single geologic unit would likely be subdivided into a series of hydrogeologic aquifers separated by several aquitards. The concept of representative values in hydrology is generally more useful at small (regional) scales to describe gross changes in material-property trends, particularly in the vertical direction. At larger scales, the idealized nature of the supposedly representative value assigned may significantly distort local heterogeneities in the rocks, and thus induce inaccuracies in the modeled flow field.

Nearest-Neighbor Approach

Another simple method related to the representative value approach, but one which attempts to consider spatial variability, is the nearest neighbor approach. In this modeling technique, each observed measurement is assumed to apply to a region extending away from the spatial position of that measurement essentially one-half way to the next data location. In other words, every unsampled point is assigned the value of its "nearest neighbor." The technique is also referred to as a *polygon method*, because the areas of influence can be determined as irregularly shaped polygons centered on each measured datum.

The nearest-neighbor approach is applicable in many of the same situations as the representative-value modeling method. The technique would be well suited for regional- to subregional-scale hydrologic models with sparse, but well-distributed measurements of hydrologic properties. At larger scales, the step-function nature of changes in material properties may introduce added complications into process (flow) computations.

Inverse-Distance Methods

Inverse-distance methods represent an effort to improve upon the discontinuous, step-function models of spatially variable properties that are generated by nearest-neighbor or polygon techniques. There are numerous variants of the method, the common denominator being that the estimated value is a weighted function of the surrounding measurements (or a subset thereof). The weights are assigned *inversely* proportional to the scalar distance from the point being estimated to the datum being considered. Thus, nearby neighboring data assume a major influence, whereas more distant neighbors assume less weight.

The general formula is:

$$\hat{Z}(x) = \frac{\sum_{\alpha=1}^{n} \frac{1}{|x - x_\alpha|^\omega} Z(x_\alpha)}{\sum_{\alpha=1}^{n} \frac{1}{|x - x_\alpha|^\omega}} \tag{2.1}$$

where $\hat{Z}(x)$ is the value being estimated at unsampled location, x, the $Z(x_\alpha)$, $\alpha = 1, 2, \ldots n$, are the available measured data at spatial locations x_α, and $|x - x_\alpha|$ represents the scalar distance from datum, x_α, to the unsampled location, x. Typically, the inverse-distance weighting scheme is nonlinear, such that the weights are an inverse function of the distance raised to some power, ω.

The square ($\omega = 2$) of the distance is most frequently assumed, leading to the terminology of *inverse-distance-squared* weighting (IDS). Other exponents are possible. The choice is relatively arbitrary, but the intended effect is to weight progressively more distant data disproportionately less than nearby observations.

Inverse-distance weighting schemes are generally assumed to be isotropic; the relative spatial position of data is not considered, only the absolute distance to the point being estimated. Geometric anisotropy could be accounted for through a rescaling of the coordinate axes. However, this is rarely implemented in practice, as there are more sophisticated weighting functions (see *Kriging*, below) that can be applied if the assumption of simple isotropic spatial variability is not warranted.

Moving Averages

Moving-average techniques are precursors to kriging methods (discussed below) and may prove useful as screening tools for examining large-scale trends. Moving averages have been used extensively to estimate block-scale properties from smaller samples (see also Section 2.2.2.4). Often, the mean value of a block is largely independent of the size of the block, once some minimum volume has been exceeded. However, it has also been shown (Desbarats and Dimitrakopoulos, 1990) that the variance of contained properties is inversely related to block size, declining as the volume of the sample actually measured increases. This relationship can lead to problems in estimating a representative effective property at the scale of, for example, a flow-model simulation grid, from measurements made on samples several orders of magnitude smaller (e.g., core samples). The variance of the core-sample properties may be so high that a realistic estimate of the block-effective property is not meaningful. To produce estimates that have less variance, we may utilize moving averages of the core-sample data to reduce the effect of samples from the extreme tails of the distribution. The technique may be particularly useful in uncovering general or regional trends than might otherwise be obscured by the mathematical effects of a few extreme values.

Like inverse-distance methods and kriging, the moving-average approach is founded on the estimation of a block or point value from a search of all neighboring data within some prescribed pattern. The search region is typically a circle of specified radius or a square implied by a limited number of grid nodes centered on the location to be estimated. In its simplest form, the moving-average technique simply computes the arithmetic mean of all observations within the desired pattern and applies that value to the estimated block. The estimate may also be based upon some weighted function of the distance. In this case, the approach is still less rigorous than kriging, because the weighting function is assumed, rather than developed from the data.

Kriging

Kriging is a relatively sophisticated extension of inverse-distance weighting schemes, in that data "close" to an unsampled location are weighted more than those values "far" away. In contrast to straightforward inverse-distance methods, kriging (and other geostatistical methods, described below) make use of weighting schemes based on a quantitative measure of spatial covariance, generally referred to as the *variogram*.

The variogram (also referred to as spatial covariance structure, spatial correlation, spatial continuity pattern, and similar phrases) is normally developed through analysis of a specific set of data. Thus, it is a measure of continuity custom-tailored to the problem at hand and not an arbitrary choice, such as the power $\omega = 2$ in inverse-distance *squared* modeling (Equation 2.1). Continuity patterns may be anisotropic, with significantly greater continuity observed in one particular direction. For example, a point 10 feet perpendicular to stratigraphic layering away from a given location may be much "farther" away geologically than a point 100 feet away but in a direction parallel to that stratification. The sample variogram, $\gamma(\boldsymbol{h})$, statistically represents the difference in value of a property among pairs of data as the vector distance, $\boldsymbol{h}$, between the members of the pairs increases. For mathematical reasons, this statistical difference is expressed in the form of a variance (Journel and Huijbregts, 1978):

$$2\gamma(\boldsymbol{h}) \equiv Var\{Z(x+\boldsymbol{h}) - Z(x)\} =$$

$$E\{[Z(x+\boldsymbol{h}) - Z(x)]^2\} = \frac{1}{N}\sum_{i=1}^{N(\vec{h})} [Z(x+\boldsymbol{h}) - Z(x)]^2 , \qquad (2.2)$$

where x is a particular spatial location, N is the number of samples, and $Z(x)$ is the value or categorical property observed at that location. $E\{...\}$ is the expectation operator and $Var\{...\}$ is the variance operator.

The variogram follows from the intuition that two sample values located close together generally are more similar than two values located further apart. The average squared difference of pairs of values separated by a given distance is *expected* to be smaller at short distances, $\boldsymbol{h}$. A specific functional relationship is fitted to the sample variogram to provide a complete description of spatial continuity in all directions and for all distances. This mathematical variogram model is described by the orientation of its major and minor axes, the range of correlation (a), the sill or absolute magnitude of the sample variance (C), and any nugget effect (C_o) representing irresolvable small-scale variability at short separation distances (Figure 2.1).

Once the spatial dependence of the various observations has been captured through variography, the variogram model is used to compute the weights to be assigned to the measurements for estimating each unsampled location in turn. The computational algorithm used in kriging

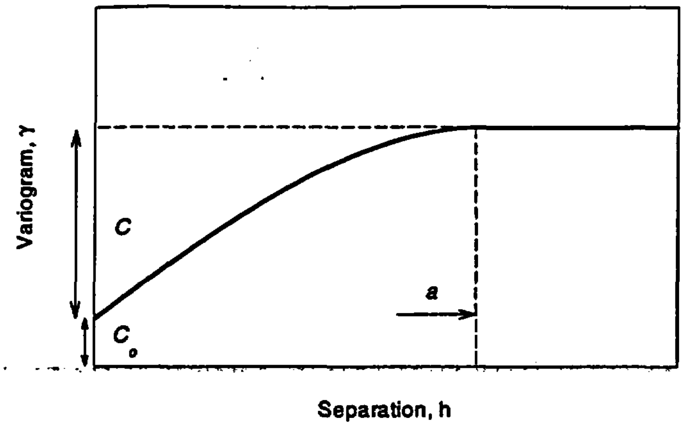

Figure 2.1 Components of a typical variogram model. *a:* range of correlation; *C:* sill; C_0: nugget effect.

largely eliminates undesirable effects of clustered data, in the sense that a group of observations preferentially located with respect to a point being estimated will collectively be assigned approximately the same weight as a single point located at roughly the same distance, but in the opposite direction. Conversely, in standard inverse-distance weighting, clustered observations may significantly skew the estimate of nearby locations.

Kriging is an exact interpolator, which means that at the location of a sampled datum, the weighting function gives back the measured value. Thus, a kriged model is "indistinguishable" from reality based on the samples themselves. However, there are generally significant departures of broader statistical measures between the observed data and a kriged model. The histogram of all values composing the model usually is quite different from the histogram of the measured data. Unless one has fortuitously sampled the actual maximum and minimum values of the variable extant in nature, the range of the histogram will be much reduced from that of the sample data. Typically, the model histogram appears more Gaussian in form than the equivalent distribution of the supporting sample data. Computing a variogram for the exhaustive kriged model generally results in a much longer range of spatial correlation. Notably, variability at short separation distances is invariably damped out, in that kriging effectively "smears" the measurements in a relatively smooth manner between sample points.

Depending upon the application of the numerical model of geology being constructed, this lack of reproduction of the univariate and spatial statistical character of the measured data may distort the ultimate physical process being modeled. For example, if high values of permeability are physically connected in space, an approach that averages-out the high values with more median values may not be conservative in the case of a ground-water flow problem. If the statistical properties of the modeled ensemble as a whole are important to the physical-process modeling to which the numerical representation of material properties are input, other geostatistical methods, such as simulation (Section 2.2.2.2), may be more appropriate.

A number of estimation algorithms based on the kriging principle have evolved over the years. All of these algorithms attempt to provide a "best," minimum least-squares error variance estimate derived from a stationary two-point covariance model. A few of the more useful kriging algorithms are discussed in the remainder of this section.

Simple kriging -- The simple kriging algorithm is given by:

$$[\hat{Z}_{SK}(x) - m(x)] = \sum_{\alpha=1}^{n} \lambda_\alpha(x)\,[Z(x_\alpha) - m(x_\alpha)] \tag{2.3}$$

where $\hat{Z}_{SK}(x)$ is the simple kriging estimator at spatial location x, the λ_α are the weights assigned to the n data, $Z(x)$, at locations $x_{\alpha=1,\,n}$, and $m(x)=E\{Z(x)\}$, the expected value of the random variable $Z(x)$. The λ_α are computed from the spatial covariances among the data and location to be estimated.

Simple kriging requires prior knowledge of the sample mean, $m(x)$, and the two-point spatial covariance developed external to the estimation process. Generally, the assumption is that the mean is constant. In most practical situations, inference of the means and covariance values requires a prior decision of stationarity of the random function assumed to control the actual physical values. If the random function is stationary with constant mean and a known covariance function, then the simple kriging estimate provides a minimized error (estimation) variance.

This minimum-error variance property of simple kriging allows it to approximate, and, under certain assumptions, to actually identify, the conditional expectation of the property being estimated. The development of an expectation and variance through simple kriging can be used to develop the underpinnings of stochastic simulation, whereby these values serve to define a conditional probability density function, from which replicate "realizations" of a material-property field may be drawn. This approach is developed further in Section 2.2.2.2, under *Geostatistical Simulation.*

Ordinary kriging -- Although simple kriging is the algorithm of choice according to strict theory of stationarity, the simple kriging estimator does not adapt to local trends in the data because it actually estimates departures from a "mean" value, $m(x)$ in Equation 2.3, that is assumed known and (generally) constant throughout the region being estimated. Consequently, if sufficient data exist to suggest the presence of trends (local nonstationarity), the more robust procedure of ordinary kriging is preferred. Ordinary kriging functionally re-estimates the local mean at each location simply by using data within the search neighborhood (effectively a moving average):

$$\hat{Z}_{OK}(x) = \sum_{\alpha=1}^{n} \lambda_\alpha Z(x_\alpha) \tag{2.4}$$

Here $\hat{Z}_{OK}(x)$ is the ordinary kriging estimator at location x, and the λ_α are the weights assigned to the n data, Z(x), at locations $x_{\alpha=1,\,n}$.

Indicator Kriging -- Indicator kriging makes use of a binary, indicator-transformed variable,

$$I(x) = \begin{cases} 1 \rightarrow Z(x) \le z_k \\ 0 \rightarrow Z(x) > z_k \end{cases} , \tag{2.5}$$

which simply evaluates whether or not the property at an unsampled location is above or below some externally specified threshold value, z_k.

The approach is considered *nonparametric* in the sense that it does not operate directly upon a few parameters assumed to define the complete probability density function of the variable of interest. The objective of indicator kriging is not to estimate the unsampled property (or its indicator transform) *per se*, but rather it provides a least-squares estimate of the cumulative distribution function of the underlying variable relative to the selected threshold value, z_k, conditioned to the neighboring data. By use of a series of such threshold values, it is possible to develop a location-specific, probabilistic model of the uncertainty associated with the value prevailing at the unsampled location. Either simple or ordinary kriging may be used to estimate the cumulative distribution function.

A variation of the indicator-kriging algorithm may be applied in instances where the variable of interest is categorical in nature (for example rock type), rather than continuous (e.g., porosity). Thus:

$$I(x) = \begin{cases} 1 \rightarrow Z(x) \in \text{Category K} \\ 0 \rightarrow Z(x) \quad \text{otherwise} \end{cases} \tag{2.6}$$

Soft Kriging -- A major advantage of the indicator-kriging approach to generating a probability estimate is its ability to consider "soft" data, or information which is known with less than certainty (i.e., the probability of the event is less than one). If the soft or "fuzzy" data can be coded as a prior local-probability estimate (e.g., as an eighty:twenty [0.8:0.2] likelihood of exceeding z_k), based upon subjective judgement or partial knowledge, indicator kriging can be used to incorporate that soft information into a posterior probability estimate. The approach builds upon the approach of Bayesian updating using information supplied by the neighboring local-probability values (Zhu, 1991).

Cokriging -- In all the estimation methods presented thus far, all estimates were derived using only the sample values of one variable. However, a data set will often contain not only a primary variable, but also one or more collocated secondary variables. Such secondary variables frequently exhibit some degree of cross-correlation with the primary variable. The existence of such cross-variable correlation poses two issues.

First, to the extent that the inter-variable correlation is a strong one, the secondary variable(s) provide potentially useful information about the primary variable. The application of cokriging (e.g., Isaaks and Srivastava, 1989) as a method of estimation aids in minimizing the estimation error in the primary variable by exploiting the cross-correlation between the primary and secondary variable(s). Cokriging requires determination of not only the spatial correlation pattern of each variable with itself, but also of each of the cross-variable spatial covariances as well (a total of k^2 variograms for k separate variables; Journel and Huijbregts, 1978). Because of the difficulty of inferring the full spatial description of the coregionalization, cokriging is uncommon, and is usually implemented only in the case where the primary variable of interest is undersampled with respect to some other material property.

Second, it is an error to estimate two correlated variables independently, as this may destroy the correlation of the variables within the model(s) and lead to erroneous or unrealistic physical-process results if the two spatially distributed fields are examined simultaneously (e.g., used as input to a flow-and-transport code). The existence of this error follows directly from the presumption that two variables (material properties) are correlated. If such cross-variable correlation exists, then for each value of one variable, there is a *conditional expectation* for the value of the other. The standard (cross-variable) correlation coefficient, usually indicated as ρ, is a measure of the spread of this conditional expectation (e.g., Larson, 1982). If two spatially correlated fields are generated without taking this joint dependency into consideration, it is possible to reproduce individually the desired spatial continuity patterns, but ρ computed across the entire field may well not approximate ρ computed for simply the data themselves. Such errors are significantly less serious in estimation, in which unsampled locations are assigned values through interpolation or smoothing of the data (which exhibit the desired cross-variable correlation), than in simulation, in which those unsampled locations are assigned values through sampling from a probability distribution. Additional discussion of the joint modeling of several variables is provided in Section 2.2.2.3.

Indicator Principal-Component Kriging -- Indicator principal-component kriging (Suro-Perez and Journel, 1991) may be used in some instances to reduce the problem of inference of multiple correlation structures. In this approach, the indicator transforms (Eq. 2.6) are themselves transformed through principal-component analysis (Davis, 1986), which orders the new variables with respect to variance and spatial correlation. The first principal component possesses the largest variance and greatest spatial correlation. The magnitude of the cross-covariances and ranges of correlation decrease significantly through the higher-order principal components. This allows approximation of the entire discretized variable by kriging only the first few (sometimes one) principal components, and performing only a simple moving-average estimation of the higher-order components. Back-transformation of the principal components at the end of the process results in the desired estimated material-property field. Indicator principal-component kriging is typically applied to the case of estimating several (K>1) categorical variables (Deutsch and Journel, 1992).

2.2.2.2 Simulation

Simulation is closely allied with the Monte-Carlo approach to evaluating uncertainty in a modeled physical process (Isaaks, 1990; Rautman and Treadway, 1991). If the material properties existing in nature are uncertain, one simply generates a large number of stochastic realizations sampled from some "likely" distribution of values and evaluates the consequences of not knowing the actual value. As with estimation, a number of alternative simulation approaches exist, each with varying degrees of sophistication.

Univariate Simulation

Simple univariate simulation consists of sampling randomly from an "appropriate" probability distribution function (*pdf*). Frequently employed distribution types include normal, log-normal, and beta functions (Kaplan and Yarrington, 1989; Kaplan, 1991). Various techniques, such as Latin hypercube sampling, are sometimes used to improve the efficiency of univariate simulation in sampling the extreme values (tails) of the probability distribution (for example, Iman and Shortencarier, 1984).

A key attribute, and a limitation, of univariate simulation procedures is that the values generated possess no particular spatial arrangement or context. As such, the process is particularly well suited as a stochastic variant of the representative-value modeling approach (see Section 2.2.2.1) for small-scale (regional to subregional) problems. Attempts to apply univariate simulation in a spatial context to larger-scale modeling problems will tend to induce illogical juxtapositions of values of the variable of interest. Intuitively, if a particular grid block is assigned a value sampled from the low-tail of the probability distribution of a variable, one would generally expect that the adjoining grid block(s) would tend to exhibit low values also. However, because univariate simulation techniques do not allow for any explicit form of spatial correlation, it is most likely that such an adjoining grid block will be simulated as approximately the mode of the distribution, and there is a significant finite probability of generating a value sampled from the opposite, high-tail of the same *pdf*. If the range of spatial correlation is significant compared with the size of the grid cells being modeled, more sophisticated geostatistical approaches are required.

Geostatistical Simulation

Geostatistical simulation comprises a large class of modeling techniques that can produce very complex, and presumably therefore highly realistic, numerical representations of spatially variable material properties. Simulation may be thought of as "expanding" (Journel and Alabert, 1989) the actual information available in a stochastic manner compatible with additional information derived from the data ensemble and the spatial context of those data. The process builds upon the geologic intuition that unsampled locations nearby a known value "tend" to resemble that value, whereas unsampled locations at increasing distances from a known value tend progressively to resemble that datum less and less. This intuition will be observed statistically in a suite of several simulations.

The philosophical framework of simulation is simple. Using concepts of random variables, one develops a model of the probability density function (*pdf*) for a material property of interest at all locations in space. By transforming the measured data to their respective positions on the probability density function and using simple kriging (see discussion in Section 2.2.2.1, Equation 2.3), the desired *pdfs* can be made conditional to a set of measured values. Alternative realizations are simply generated by sampling from these *pdfs*. The variance of individual, location-specific, *pdfs* will vary with the amount of geologic uncertainty. Near conditioning data (Figure 2.2(c)), the *pdf* associated with an unsampled location will be relatively narrow. Where less information is known, such as away from data or in the vicinity of conflicting measurements, the *pdf* will be relatively broad (Figure 2.2(a-b)), leading to generation of a wide range of likely values across a suite of realizations. Because the underlying kriging algorithm used to derive the *pdfs* is an exact interpolator, the *pdf* degenerates to a spike with probability = 1 at a measured location (Figure 2.2(d).

Simulations may be conditional or nonconditional. Conditional simulations are numerically anchored to a specific set of real-world data (as described in the preceding paragraph), and they possess three special properties that add to their usefulness in evaluating the effects of geologic uncertainty on physical process models. Specifically, conditional simulations:

1. reproduce the known data values at the same locations within the model as represented by the real-world samples;

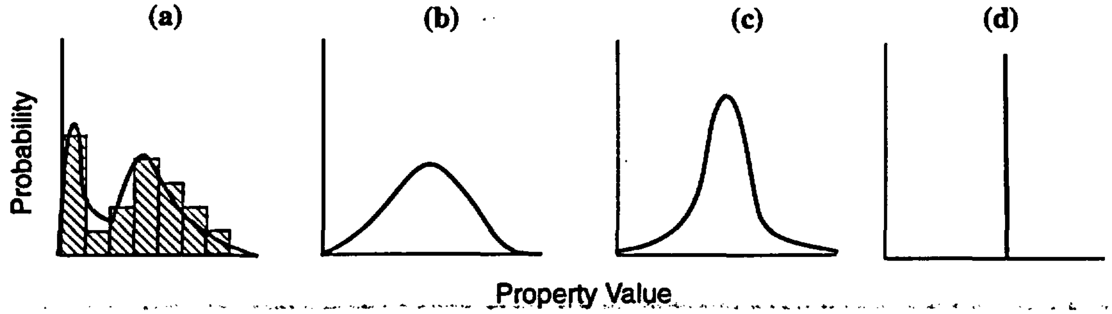

Figure 2.2 Conceptual probability density functions representing the uncertainty associated with various unsampled locations. (a) Beyond the range of spatial correlation: *pdf* is virtually identical to the univariate histogram; essentially all that is known about the unsampled location is what is known about the population as a whole. (b) Far away from a sample, but within the range of spatial correlation: *pdf* is broad, indicating considerable uncertainty; distribution begins to focus on expected value. (c) Nearby a sample value: *pdf* is narrower indicating lesser uncertainty. (d) Immediately adjacent to a sample value: *pdf* is nearly a spike value corresponding to the adjacent sample datum.

2. reproduce the overall univariate descriptive statistics of the known data values; and
3. reproduce the bivariate statistics, or spatial correlation structure, of the data.

Unconditional simulations are similar, except that they are not conditioned to any particular spatially anchored data, and thus item 1 does not apply. As simulations with these characteristics cannot be distinguished statistically from the ensemble of data used in their construction, they serve as alternative, equally-likely stochastic realizations of an incompletely sampled and measured reality.

Simulations may also be developed using parametric or nonparametric techniques for mechanically inducing the desired univariate (item 2 above) and bivariate statistical properties (item 3). Parametric techniques rely upon the predictive power of well-understood multivariate probability functions, almost invariably the multivariate Gaussian. A large number of algorithms have been developed that implement Gaussian-related simulation (for example, references in Deutsch and Journel, 1992).

Nonparametric techniques have been developed to deal with some of the inherent limitations of the multivariate Gaussian probability functions. Most notable among the nonparametric approaches is the indicator method (Journel, 1983; see also equation (2.5)). Because nonparametric methods require explicit development of the complete, spatially correlated probability density function from the data, the approach is data- and computationally intensive. However, if the data indicate that the spatial behavior of values in the tails of the distribution is significantly different from that predicted by Gaussian theory (for example, Journel and Alabert, 1989; Rautman and Treadway, 1991), there may be little alternative if the spatial continuity of these potentially very important extreme values is to be modeled correctly. Nonparametric methods are also appropriated for the simulation of categorical variables, such as lithology (Rautman and Robey, 1994).

Advanced Simulation of Spatially Correlated Variables

A theoretically separate technique for producing simulated fields of spatially varying values makes use of an optimization method known as *simulated annealing* (Kirkpatrick and others, 1983). Named for the metallurgical process, simulated annealing in this context involves creating an initial random field with the proper univariate statistics (proportions of values). Pairs of values are then swapped at random (thus not changing the overall univariate properties of the field). Swaps that lower the computed value of some objective function, which measures the closeness of the actual field to some desired criterion, are retained whereas swaps that raise the value of the objective function are generally rejected. The "annealing" analogy enters, in that early in the swapping process (i.e., at high temperatures in the annealing of metals), some swaps are accepted even if they increase the objective function; this is allowed to enable the annealing process to escape local minima and converge to an overall better match to the desired criterion. Later in the process (at lower temperatures), the probability of accepting such disordering swaps is progressively reduced.

To the extent that the objective function selected is a variogram-like measure of two-point spatial continuity, simulated annealing is essentially a "geostatistical" method, although one not based on any variant of kriging. However, other objective functions can be defined. It is possible to define three-, four-, or arbitrarily multiple-point continuity measures which are to be induced in the annealed model. Theoretically non-colinear continuity could be induced, such as is associated with cross bedding in sandstones. Most practical applications of simulated annealing has focused principally on replication of a desired two-point variogram model in the output realizations (Deutsch and Journel, 1992).

2.2.2.3 Joint Modeling of Several Variables

Numerical modeling of physical processes generally requires as input more than one material property. For example, TOSPAC, one of the current principal total-system performance assessment flow-and-transport codes, requires as input seven separate material properties for the rock matrix and ten properties for the fractures (Dudley *et al.*, 1988). It is almost certain that some, if not many of the individual properties required as input to the physical process models supported by the Three-Dimensional Rock Characteristics Models Study are not independent, but rather are correlated to some extent with one another. A prominent example of such correlation is that between matrix porosity and permeability in welded tuffs (e.g., Rautman *et al.*, 1993).

If two variables are both correlated one with another and spatially variable, then it is a distortion of reality to model the spatial distribution of such properties independently. This statement is particularly relevant with respect to geostatistical simulation (Section 2.2.2.2). As indicated in the section on *Kriging*, the existence of cross-variable correlation implies that the conditional expectation of one variable is a function of the other. Because simulation generates values at unsampled locations by random sampling from a pdf, it is important to use the proper, *conditional* pdf, rather than the overall (univariate) pdf. Depending upon the extent of the correlation and the use of the specific variables within the subsequent process-modeling, significant distortions of real-world physical-process behavior may result.

The solution is the joint spatial modeling of several variables. Most simulation algorithms theoretically can be generalized to produce such joint realizations. The difficulty, however, resides in the inference and modeling of the cross covariances between the variables. Computational time is a real, although subsidiary, consideration. For these reasons, joint simulation of several variables is rarely implemented directly. Rather, pragmatic approximations are adopted that limit the influence of spatially collocated, logically inconsistent material properties.

The principal simplification is to simulate the most important (to the subsequent process model) or most strongly correlated variable independently. In turn, other covariates are simulated by drawing from their specific conditional distribution, given the value of the first variable, at each location. The necessary conditional distributions are inferred from the scattergram of the two variables; the sampling may be conducted with or without consideration of the strength of the correlation (i.e., with or without added "noise"). In this simplification, spatial autocorrelation is induced in the secondary variable indirectly through that of the primary variable. Rautman and Robey (1993) presented an example of this method of joint simulation, wherein porosity values were first simulated from conditioning data. Saturated conductivity values were then generated from the porosity-conductivity regression line. Normally distributed variability was subsequently added to the predicted conductivity value, sampled from a distribution with the appropriate standard deviation.

Another approach to the joint simulation of several variables, primarily categorical variables such as rock type, is indicator principal-component simulation (Deutsch and Journel, 1992). Indicator principal-component simulation is an extension of the indicator principal-component kriging approach (see page 20), in that the multiple variables are first transformed through principal-components analysis (e.g., Davis, 1986) into a new vector of principal components. Because the majority of the spatial continuity of the joint variables is captured in the first principal component, direct kriging of this transformed variable produces a spatially correlated field, which serves as the basis for the local, conditional, indicator cumulative distribution function (*cdf*). The remaining principal component variables tend not to be spatially correlated. The local *cdf*s are then used, as in all other simulation techniques, to constrain the outcome of a simulated values generated by random drawing.

New approaches to Gaussian simulation (Xu *et al.*, 1992; Almeida, 1993), in which the cross-covariance relationships between two *collocated* variables are greatly simplified through what is known as the "Markov-Bayes" approximation, may prove to be of significant utility in the joint modeling of two variables. In the simplest sense, the Markov model makes use of the hypothesis that a collocated primary datum effectively screens the influence on a secondary variable of any primary data located at a distance. This negates the need to develop a model of the cross-covariance between primary and secondary variables at any separation distance other than zero. The covariance at separations equal to zero is identified simply through the cross-variable correlation coefficient (Xu *et al.*, 1992). The downside of this enabling hypothesis is the requirement for the availability of the secondary variable at all locations for which a simulation of the primary variable is desired.

2.2.2.4 Scaling Issues

When modeling heterogeneous material properties, it is important to consider the scale at which the conditioning measurements were made in comparison with the scale at which the models will be applied (*measurement support*, in geostatistical jargon). Although some material properties to be modeled by the Three-Dimensional Rock Characteristics Models Study average, or scale-up, in an arithmetic sense (notably compositional properties and porosity), it is not generally possible to represent exactly large-scale effective material properties, such as hydraulic conductivity, by simple linear or nonlinear combinations of smaller-scale measurements. Confounding the issue is that it is generally impractical to make measurements on volumes that are comparable to the volume-element scale required for physical-process modeling of regional hydrogeologic flow systems or even of smaller, engineered structures, such as a mined repository opening.

Most physical-process models are based on a continuum approach. This involves replacing an actual heterogeneous medium, which may contain discrete discontinuities, by a fictitious continuum, in which the physical properties, locally averaged over some "representative-elementary volume," vary continuously in space. For example, the partial differential equations governing fluid flow are often obtained by expressing the required conservation of mass, momentum, and energy at the scale of the volume-averaged material properties.

Difficulties arise when the representative-elementary volume cannot be defined or can only be defined as large compared with the scale over which the analysis or test is performed. Typically in these cases, some new physical process or mode of behavior appears as the scale of the observation changes. For example, if the material property variable required for the solution of a particular process-response modeling exercise depends upon the geometry of scale in which the analysis is posed, that variable is not an intrinsic property of the material in which the process operates. Rather, the "property" may be conditional upon secondary properties or on geometric orientation. This type of dependence is seen in permeability or hydraulic conductivity with relationship to Darcy's Law for flow in porous media. At scales below the representative elementary volume, the intrinsic permeability of a porous solid is dependent upon both the direction of flow and the location of observation. Fluid elements within a porous medium follow a tortuous path much greater than the macroscopic distance between two points. These paths, and consequently determinations of permeability, obviously will be different if flow is considered parallel versus normal to bedding geometry, or radial to some screened well interval in three dimensions. Another instance involves the effects of scale on rock strength and deformation modulus. As the scale increases to a representative rock mass (volume), the strength and deformation modulus will decrease. A small intact volume of rock with no fractures will have a greater strength and deformation modulus than a larger volume of rock, which will probably contain fractures (discontinuities).

Specific approaches to addressing scaling issues within this Study Plan are difficult to define. This difficulty is partly because most modeling activities are *ad hoc*, and scaling techniques must be closely aligned with the ultimate use of the rock characteristics models. Additional difficulty arises because there are few good, well-accepted approaches to the scaling of the more difficult hydrologic properties. Frequently, the problem is simply ignored and process modeling is conducted using point values for these properties.

Abundant theoretical and practical experience is available from the mining literature, which allows prediction of changes in the statistical distribution of reported values as a function of the support volume over which those values are measured (David, 1977; Journel and Huijbregts, 1978; Clark, 1979). For material properties that average arithmetically, the mean of the distribution does not change with scale, and the variance of the population decreases in a predictable manner as the relative support volume increases. The class of arithmetically averaging material properties includes virtually all compositional variables (mining "grades") and most of the "bulk" properties of a rock mass (e.g., porosity, density).

In estimation modeling (i.e., kriging), change of support is typically implemented (for appropriate properties) in a location-specific setting simply by estimating an array of points within the desired volume and assigning the arithmetic average of those points to the larger volume. A similar approach could be applied to simulated models; however, most frequently, the purpose of simulation is to investigate small-scale variability. Volume-averaging over large blocks would obscure most of this variability, thus negating the advantages of simulation as a modeling technique. Nevertheless, simple volume averaging of very fine-mesh simulated points might be a practical method of upscaling appropriate measurements slightly.

The scaling of permeability-type measurements, which do not average arithmetically, is the focus of a relatively active research specialty (e.g., Tidwell, 1994), and a number of possible solutions have been proposed. For example, block-scale effective permeabilities for certain sand-shale sequences in petroleum applications have been effectively generated using the permeability of the sand and the sand/shale ratio (Journel et al., 1986; Desbarats, 1987; Deutsch, 1987). The relationship appears to be largely empirical, and thus location-specific. The approach appears contingent upon the existence of a bimodal (permeable/non-permeable) lithologic environment in which the two lithologic types are intimately intermixed on the scale of the final, modeled blocks. This appears not to be the case at Yucca Mountain generally, although the technique might be applicable to specific problems of smaller extent.

A second major published approach has been to use process-modeling (i.e., flow) codes to generate the equivalent effective permeability values for a number of large blocks comprised of smaller-scale property values. These large-block values are properly distributed in the overall model volume, and the complete model is then directly generated stochastically from the geostatistical properties of the block-scale values (Rubin and Gomez-Hernandez, 1990; Gomez-Hernandez, 1992). The direct-simulation approach is computationally and labor intensive, and it is further limited by the requirement that the direction of the overall fluid flow be known and constant.

A third approach to scaling permeability data is again a pragmatic one similar to the empirical averaging technique. Rautman and Robey (1993) attempted to minimize problems associated with arithmetic averaging of (frequently) widely varying permeability values by using an adaptive gridding approach that minimized the within-block variability. Jensen (1991) adopted a computationally much simpler, but conceptually somewhat similar, approach employing merely the geometric mean of the contained small-scale data. The novel aspect of this method is that a percentage of values in both tails of the within-block distribution were discounted to some extent, yet were not simply truncated (and thus ignored). In this manner, a few very-extreme small-scale values would not "drive" the result of the geometric average, as in the usual, uncorrected case, and the "average" is more centered. The difficulty of both these approaches is that the pragmatic simplifications made in the name of computational feasibility may not adequately reflect actual flow paths. If the extreme values within a given grid block are highly connected, the effective permeability of the block is in no manner an "average" of any type, but may approximate the extreme few percent of the overall distribution.

2.3 Anticipated Direction of Modeling Activities

A fundamental premise of this Study Plan is that rock characteristics modeling is very closely tied to, and narrowly aligned with, use of the resulting model(s) in subsequent physical-process modeling. This *ad hoc*, or "specific-to-the-purpose" nature of most of these modeling activities renders generalizations somewhat imprecise. However, previous experience in creating preliminary three-dimensional rock characteristics models for use on the Yucca Mountain Project allows some discussion of the anticipated direction of modeling activities. The discussion which follows is intended to be descriptive of experience to-date, and not necessarily to be prescriptive for the future. Although there is no reason to believe that this conceptual and methodological approach is not applicable to future modeling activities, this discussion should not be construed to proscribe adoption of other approaches that may be better suited to the modeling of a specific problem.

2.3.1 Conceptual and Methodological Approach

The overall conceptual framework currently guiding the development of preliminary three-dimensional rock characteristics models is illustrated in Figure 2.3, which has been framed in the context of one specific regulatory requirement for a high-level nuclear waste repository, viz. the 10 CFR 60 ground-water travel time specification. As such, the figure reaches "backward" (section 2.4.1) to the acquisition of data (the shaded dots that represent different values of a particular material property), and "forward" (section 2.4.2) through the physical-process modeling of ground-water flow (the "transfer function" or flow code), and the regulatory evaluation of uncertainty associated with the distribution of travel times (the cumulative distribution function).

Understanding the purpose of the process-modeling exercise and the regulatory criterion being addressed is critical in determining the specifics of the rock-characteristics modeling process. Even the material property(ies) to be modeled is largely dependent upon the ultimate use of the material properties model. Although any material property that can be used as input to a physical-process modeling computer code is a candidate for rock characteristics modeling under this study, there may be little benefit in creating detailed spatially variable models of a material property to which the physical process under investigation is relatively insensitive. For example, bulk density presumably has only minor impact on modeled flow of ground-water. However, this same property may have a major influence on the conduction (flow) of heat through the rock mass away from thermally hot spent fuel cannisters. Thus, the fundamental modeling decision of the variable of interest can be seen to be situation (i.e., user) specific.

Preliminary rock characteristics modeling to-date has tended to emphasize material properties of hydrologic interest. Much work, particularly that directed toward understanding the spatial correlation patterns present in volcanic tuff, has focused on porosity, a widely measured "framework" material property that has been demonstrated to be correlated with other hydrologically significant properties (L. E. Flint, USGS, written communication, 1993; Istok *et al.*, 1994) across a wide range of Yucca Mountain lithologies. In some cases, porosity has used as a modeling surrogate for the property of primary interest (Longenbaugh *et al.*, 1994). Rock type has also been modeled directly using techniques described in this Study Plan, and material properties

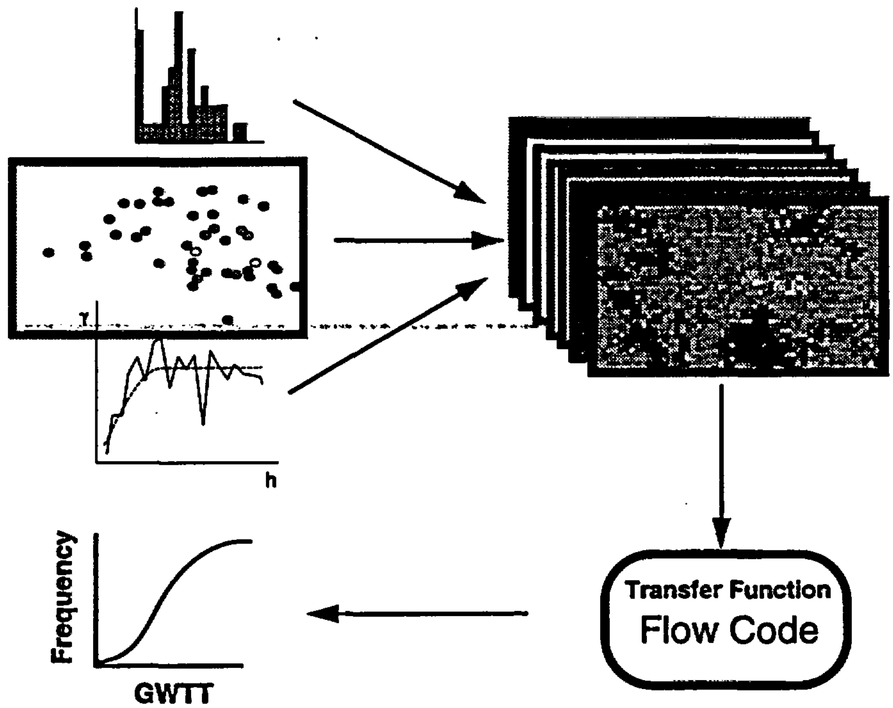

Figure 2.3 Conceptual visualization of rock characteristics modeling and uncertainty assessment proposed for the Yucca Mountain Project. Scattered data and corresponding histogram and variogram are used to generate alternative, geostatistically indistinguishable stochastic images, which are processed through a transfer function to propagate characterization uncertainty as it affects a performance measure (GWTT = ground-water travel time). Modified after Journel, 1989.

assigned after-the-fact to these stochastic rock types (Wilson *et al.*, 1994).

The remainder of the diagram, particularly those items portrayed in the upper portion, represents schematically the modeling activities of this Study. These modeling activities, simply stated, will follow a progression involving the specification of some geometric framework in which to map the data (the center left-top box) followed by in-filling of that framework with material properties values (to produce the exhaustive model(s) shown in the top right portion of Figure 2.3).

The geometric framework may be explicit (i.e., sample data locations are specified directly in a real-world coordinate system, such as Nevada State Plane), or it may be only implied during the actual modeling and imposed after-the-fact on a non-real modeling-coordinate system. Although this latter method appears complicated at first, the use of coordinates normalized in some manner to the range of zero-to-one is actually quite simple and has been widely applied in numerous applications (Journel and Gomez-Hernandez, 1989; Rautman 1990; Rautman *et al.*, 1993). A typical implementation may assume real-world coordinates in x and y, while at the same time scaling the z-dimension in stratigraphic coordinates from zero (the bottom of a unit of interest) to one (the top of that unit). Rautman *et al.* demonstrated the applicability of such stratigraphic coordinates in ash-flow tuffs to compensate for gradual changes in depositional thickness related to distance from the source vent.

The geometric framework may be extremely simple, as in a two-dimensional areal distribution of thickness-averaged properties (e.g., Figure 2.3), or it may be quite complicated in three dimensions. Some modeling problems may be addressed through subdivision of the rock column into a number of stratigraphic (or stratiform) units, probably representing some level of aggregation of the geologic subdivisions given in Figure 1.2. Material properties or other rock characteristics then would be modeled separately within each selected rock characteristics unit. Alternatively, certain issues involving uncertainty may be better addressed by ignoring stratigraphic classifications *a priori*, and letting the modeling algorithm dictate the distribution of rock types and/or material properties in a manner consistent with the data and the observed spatial continuity pattern(s). Rautman and Robey (1994; also Wilson *et al.*, 1994) attempted to address characterization uncertainty in the spatial distribution of basic rock types at Yucca Mountain in this manner. Rautman and Flint (1992) present an expanded discussion of some of the philosophical, logistical, and computational issues involved in determining the overall modeling approach in light of the geologic framework of Yucca Mountain.

Development of the material properties in-fill of a modeled volume probably will follow a relatively set sequence of steps and methods, again captured schematically in Figure 2.3. First, the statistical character of the actual data must be understood (histogram in Figure 2.3). Spatial continuity analysis is required to identify spatial correlation patterns and to develop the simplified mathematical conceptualization of that pattern (the variogram in Figure 2.3). In some cases, various combinations of soft data, geologic intuition and even surrogate or auxiliary data sets (Rautman and Robey, 1994) may be necessary to derive a believable spatial model.

At this time, geostatistical simulation is believed to be more generally useful than estimation for Yucca Mountain applications; this is represented in Figure 2.3 by the multiple stochastic images of the same data. This preliminary choice is specifically related to regulatory emphasis on uncertainty assessment and to the go/no-go nature of a decision regarding construction and licensing of a potential repository (Rautman and Treadway, 1991). Parametric (e.g. Gaussian) simulation would be the methodology of choice for the simulation of continuous variables (e.g., porosity, conductivity), unless exploratory data analysis indicates that the assumption of multivariate Gaussian spatial correlation behavior is violated. This can be determined partially by computing indicator variograms for the median and extreme (perhaps first- and third-quartile; ideally perhaps tenth and ninetieth percentile) values separately, and comparing the spatial continuity of those fractions of the overall data to the symmetrical and regularly decreasing (away from the mean) continuity patterns theoretically expected for a multivariate Gaussian distribution of similar univariate mean and variance. (Deutsch and Journel, 1992). Nonparametric approaches involving multiple indicator coding of the original continuous variable would be applicable if the spatial behavior is distinctly non-Gaussian (Journel and Alabert, 1989). Indicator methods are also the simulation methodology of choice for dealing with categorical variables such as rock type (e.g., Rautman and Robey, 1994) or the presence/absence of a specific type of alteration.

Once the necessary model(s) of the variable of interest have been generated, some type of uncertainty assessment generally would follow, for at least qualitative use in evaluating the reliability of the models themselves. In some cases, probability maps (Rautman, 1993) derived from post-processing a large number of simulations may be the most appropriate manner of evaluating the uncertainty associated with a particular model. The more complete and regulatorialy rigorous method of uncertainty assessment is portrayed in the bottom portion of Figure 2.3. The uncertainty resulting from less-than-exhaustive sampling and characterization of the site is propagated through the appropriate transfer function to reflect a distribution of some measure of site performance, here shown as ground-water travel time. This forward propagation of geologic uncertainty through model-evaluating activities (section 2.4.2) obviously requires the close interaction of this Study with those "end-user" organizations and activities (see also Tables 3.1 and 3.2). It is the requirements of these users that drive modeling under this Study Plan, and which therefore account for the repeated specification that three-dimensional rock characteristics modeling is inherently *ad hoc* in nature. The relationship of this Study to other Yucca Mountain Project activities is discussed in more detail in section 2.4.

2.3.2 Computer Software Considerations

It is not possible to provide an exhaustive list of computer software that may be used for material-properties modeling on the Yucca Mountain Project. Computing environments and modeling algorithms continue to evolve, as do the requirements for specific types of numerical property models. However, there are a number of existing software packages and other computer programs that can be used to create models, such as have been described in section 2.2.; a non-exhaustive listing is presented in Table 2.3. Previous experience in creating preliminary material-

Table 2.3 Major Computer Software Packages Available for Material-Properties Modeling

Purpose of Modeling	Package Name; Brief Description of Software	Vendor
Geometric Modeling	Lynx Geotechnical Modeling System (GMS): The Lynx GMS is a comprehensive, 3-D, volume-oriented modeling package, which allows the use of considerable geologic intuition and a diverse suite of data types to create geometric models of geology. The package contains integrated routines for modeling material properties or other attributes of the rock mass using geostatistical and other estimation algorithms.	Lynx Geosystems, Inc. Vancouver, B.C. Canada
Estimation	Lynx Geotechnical Modeling System (GMS): The Lynx GMS provides comprehensive, integrated routines for creating gridded models of material properties and other rock attributes using ordinary kriging, universal kriging, and inverse-distance-to-a-power modeling	Lynx Geosystems, Inc. Vancouver, B.C. Canada
	GSLIB: A comprehensive set of computer routines for estimation modeling, including simple, ordinary, and indicator kriging methods. Also provides implementation of more exotic types of estimation, such as universal kriging [kriging with a trend], nonlinear [disjunctive] kriging, cokriging, and indicator principal components kriging).	Stanford University Stanford, Calif.

Table 2.3 Major Computer Software Packages Available for Material-Properties Modeling

Purpose of Modeling	Package Name; Brief Description of Software	Vendor
	Geo-EAS: A user-friendly, menu-driven system for performing basic geostatistical analyses, including simple and ordinary kriging of points or of scaled-up volume-averaged blocks.	U.S. Environmental Protection Agency Las Vegas, Nev.
	ISATIS: An integrated geostatistical and geographic information systems modeling package, including routines for geostatistical (simple and ordinary kriging with several variants [kriging with a trend, intrinsic random functions of order-k, cokriging], inverse-distance-to-a-power, spline, moving averages, polygon-of-influence and other types of modeling.	Geomath Houston, Tex.
Simulation	GSLIB: A comprehensive set of computer routines for simulation modeling, including both Gaussian and indicator methods (for continuous and categorical variables). Some simulation methods are implemented using more than one algorithm (e.g., sequential, turning bands, and LU decomposition approaches to Gaussian simulation. Includes a program for simulated annealing used both as a simulator and to post-process simulations generated with other techniques.	Stanford University Stanford, Calif.
	ISATIS: An integrated geostatistical and geographic information systems modeling package, including routines for both Gaussian, indicator, and fractal simulation	Geomath Houston, Tex.

property models has let to tentative selection of the software developed by Lynx Geosystems and Stanford University. These programs may be replaced or supplemented by other packages determined to be more appropriate for any particular analysis.

Because past experience has led to emphasis on geostatistical simulation, and in particular on the GSLIB software library (Deutsch and Journel, 1992), an expanded description of the components of this library is provided in Table 2.4. Virtually all major components of a geostatistical analysis can be accomplished using this set of programs.

Table 2.4 Major Components of the *GSLIB* Geostatistical Library (Deutsch and Journel, 1992)

GSLIB Sub-library	Major Function
GAMLIB	Variogram (spatial continuity) analysis and modeling in 2-and 3-dimensions

Table 2.4 Major Components of the *GSLIB* Geostatistical Library (Deutsch and Journel, 1992)

GSLIB Sub-library	Major Function
KRIGLIB	Conventional and indicator kriging and cokriging (interpolation) algorithms in 2- and 3-dimensions; also advanced interpolation algorithms including indicator principal-components kriging and soft kriging.
SIMLIB	Monte-Carlo-style generation of spatially correlated stochastic fields using a variety of gaussian-related algorithms, indicator methods, boolean techniques and simulated annealing.
POSTPLOT	Postscript® display routines for exploratory data analysis and mapping/plotting results of geostatistical analyses
Utility Routines	Miscellaneous data transformations, post-processing algorithms, equation-solvers.

2.4 Relationship to Other Studies

As an integrative study that is intended to synthesize a wide variety of site characterization data and general geologic information to create comprehensive, coherent models of the distribution of material properties distributed in space, the relationship of the Three-Dimensional Rock Characteristics Models Study to other Yucca Mountain Project activities is complex. To some extent, the relationship is iterative, as well, because modeling of material properties inevitably will highlight inconsistencies in the input data or lead to the identification of regions within the site for which data appear insufficient. This feedback loop to data-providing field and laboratory studies is portrayed schematically in Figure 2.4. In similar fashion, the use of the numerical models of material properties produced by this Study inevitably will result in problems for the using performance-assessment and design-evaluation activities. Because these activities are the customers of this Study and directly specify the content and substance of the rock characteristics models, an additional feedback loop is established (Figure 2.4). In order to be effective, these feedback loops must operate in near-real time.

A second type of feedback loop is also shown in dotted lines on Figure 2.4 below the direct loops between this Study to its suppliers and from its customers. This loop is intended to represent a more direct, non-filtered feedback between an "end user" (such as performance assessment) and a lower level "data producer" (such as a site-characterization activity). This type of feedback might originate if an analysis activity identifies an entirely new type of data that should be sought in the field. Alternatively, ongoing site characterization might identify the operation of a heretofore unsuspected physical phenomenon that could affect the type and nature of performance or design analyses being conducted. Thus, the loop is shown operating in both directions. The exact mechanism of this form of feedback is only poorly defined, and would unquestionably be situation-specific. However, it is anticipated that "discoveries" of this type would be relatively significant, affect the entire repository program, and that the Project management structure is sufficiently flexible to accommodate the required changes.

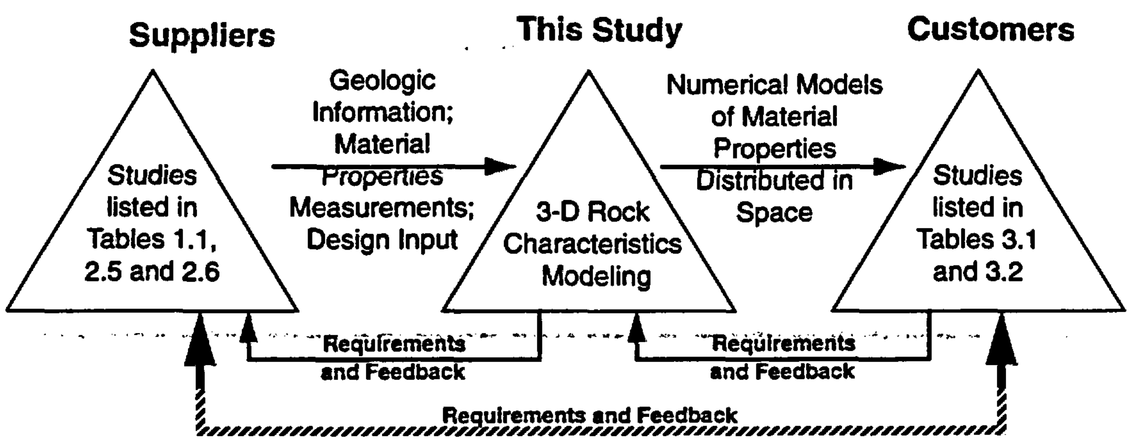

Figure 2.4 Customer-supplier model showing conceptual relationship of the Three-Dimensional Rock Characteristics Models Study to other activities described in the Site Characterization Plan

2.4.1 Data-Providing Studies

Virtually any site characterization study described in Section 8.3 of the SCP can serve as a data-providing study to the Three-Dimensional Rock Characteristics Models Study. Much of the site characterization data ultimately to be incorporated into the models will originate with field investigation programs (Table 1.1), including the various drilling efforts at Yucca Mountain (Table 2.5). Additional information will derive from mapping and other activities to be conducted within the underground workings of the Exploratory Studies Facility. Laboratory testing programs will provide quantitative measurements of various material properties, from which the spatial correlation patterns, histograms, and other information necessary to create comprehensive numerical models of those properties will be derived (Section 2.2). A non-exhaustive, but representative, listing of some of these more laboratory-oriented studies is provided in Table 2.6.

Studies obtaining large-scale field measurements, typically by performing some type of in-situ testing (e.g., hydrologic pump tests), are a unique type of "data-providing activities." The scale and cost (monetary, temporal, and logistical) of conducting large-scale field testing activities conspire to limit severely the number of locations that can be so tested. Thus, the "physical-property measurements" obtained by these types of studies almost certainly will be too sparse to support *direct* modeling of these data in the manner assumed for this Study. This is unfortunate, in that it is large-scale, effective material properties (see section 2.2.2.4) that are desired by the end-user analytical activities (section 2.4.2). Although it will probably be impossible to use the measurements produced by field-scale testing activities in the same manner as laboratory measurements and other types of more "point-like" field observations, the existence of field-test results offers one additional means of checking the realism of the material-properties models created under this Study Plan (see section 2.5.5).

Table 2.5 Summary Description of Drilling Programs Described in the SCP

SCP Drilling Program	Brief Description	Hole No.
Systematic Drilling Program; Study 8.3.1.4.3.1	The Systematic Drilling Program consists of an initial set of 12 SD- prefix holes. Some holes provide areal coverage of the repository block; others provide in-fill detail for geostatistical purposes.	SD-1 through SD-12
Unsaturated Zone Percolation; Study 8.3.1.2.2.3	The UZ Percolation Drilling Program consists of approximately 17 holes to be drilled, redrilled, or deepened. Some 11 UZ- prefix holes have been located adjacent to the repository block to provide additional data for geostatistical purposes.	UZ-2, -3, -4 -5, -7, -9, -9a, -9b, -11, -12, -14, -16
Saturated Zone Flow System; Study 8.3.1.2.3.1	The Saturated Zone Program will drill a single H-series hole for pump testing and hydrologic monitoring. The study will also drill 8 WT- series holes for better definition of the regional potentiometric surface. Hole H-7 and two of these WT- holes (WT-8 and WT-9) are located adjacent to the repository block to provide additional data for geostatistical purposes.	H-7 WT-8 WT-9
Exploration Program (for soil and rock properties at surface facilities) Study 8.3.1.14.2.1	A large number of shallow core holes are proposed at intervals along the alignment of proposed access ramps to the underground facilities	NRG-1 thru 7 SRG-1 thru 5
Vertical Seismic Profiling; Study 8.3.1.4.2.2.5	One VSP- prefix borehole is planned for instrumentation related to vertical seismic profiling studies. This hole has been incorporated into the site-coverage pattern for geostatistical purposes.	VSP-1 (now UZ-16)
Stratigraphic Studies; Study 8.3.1.4.2.1	Three additional G-series holes are planned to acquire regional stratigraphic information. These holes are located too far from the repository block to provide much geostatistical data. However, qualitative and interpretive information from these holes will be incorporated as warranted.	G-5 G-6 G-7
Mineralogy, Petrology, and Chemistry of Transport Pathways Study 8.3.1.3.2.1	One G-series hole is planned to obtain samples of deep geologic units for geochemical analysis. See notes on G- series drill holes.	G-8
Characterization of Volcanic Features Study 8.3.1.8.5.1	Four V- holes are planned to investigate four aeromagnetic anomalies that may represent buried volcanic or intrusive features to the west of the site. See notes on G- series drill holes.	V-1, V-2, V-3, V-4

Table 2.6 Partial listing of laboratory studies that may produce material property measurements for developing three-dimensional models of rock characteristics.

SCP Study	Participant	Material Properties Measured
		Bulk Properties
8.3.1.2.2.3	USGS	bulk density: dry, saturated
"	"	particle density
"	"	porosity
8.3.1.4.3.1	Sandia	bulk density: dry, saturated
"	"	particle density
"	"	porosity
8.3.1.15.1.1	Sandia	bulk density: dry, saturated
"	"	grain density
"	"	porosity
8.3.1.14.2.2	Sandia	density
"	"	porosity
		Hydrologic Properties
8.3.1.2.2.3	USGS	water content: gravimetric, volumetric
"	"	saturation
"	"	water potential
"	"	matrix permeability: water saturated
"	"	matrix permeability: gas saturated
"	"	relative permeability
"	"	moisture retention relations
8.3.1.4.3.1	Sandia	water content: gravimetric, volumetric
"	"	saturation
"	"	matrix permeability: water saturated
		moisture content
		Thermal Properties
8.3.1.15.1.1	Sandia	heat capacity
"	"	thermal conductivity
8.3.1.15.1.2	"	coefficient of linear thermal expansion
		Mechanical Properties
8.3.1.15.1.3	Sandia	unconfined compressive strength
"	Sandia	Poisson's ratio
"	"	Young's modulus
8.3.1.15.1.4	"	fracture normal stiffness
"	"	fracture shear stiffness
"	"	fracture cohesion
"	"	fracture coefficient of friction
"	"	fracture surface roughness
8.3.4.2.4.3	LLNL	unconfined compressive strength
"	"	shear strength
"	"	fracture normal stiffness
"	"	fracture shear stiffness
8.3.1.14.2.2	Sandia	fracture surface roughness
		Geochemical Properties
8.3.1.3.2.1	LANL	mineralogy

2.4.2 Model-Evaluating Activities

The three dimensional models of rock characteristics developed under this Study will be used in various design-evaluation and performance-assessment activities. Because of the structure of the Site Characterization Plan, these activities are not formally classified as "studies." However, the relationship of this Study to those activities is functionally the same as if they were formal studies.

Because this Study will produce rock characteristics models to meet the requirements of specific design-evaluation and performance-assessment activities, the models generally will be custom-constructed to the specifications of the end-user activity. Because of this critical, direct linear relationship, expanded discussion of the relationship between this Study and design evaluation and performance assessment is the focus of Section 3.0, *Application of Results*.

2.4.3 Similar Intermediate Modeling Studies

The Three-Dimensional Rock Characteristics Models Study is in an "intermediate" position with respect to the overall modeling efforts of the Yucca Mountain Project.[1] At a lower level and directly related to site-characterization activities, there is modeling of a type conducted to convert raw measurements of voltages, pressures, volumes, and similar direct physical measurements to more generally useful material properties (or rock characteristics). Some of this "modeling" may be quite sophisticated. At a higher level, there is physical-process modeling conducted at various levels of detail to address such summary processes as the functioning of the overall regional hydrologic flow system or the cumulative releases of radionuclides to the accessible environment over some stated period of time. There are other studies that will produce similar, intermediate-level models. Thus, it appears appropriate to discuss the relationship of this Study to other intermediate modeling studies.

Figure 2.5 is a conceptual flow diagram of the relationships among the various "levels" of modeling on the Yucca Mountain Project. At the base of the diagram are site-characterization data-providing activities (Section 2.4.1) that acquire various types of raw data and generally conduct some form of modeling to reduce those data to numerical material properties. The degree of data integration at this level is relatively low, and each physical process represented is essentially modeled at the fundamental, constitutive level of detail. At the top of the diagram, representing a very high level of data integration and both data and physical-process abstraction, are model-evaluating activities (Section 2.4.2). These high-level activities model the functioning of a particular physical process (perhaps coupled processes) and provide an understanding of the physical system at a physical scale on which an evaluation of suitability may be made with respect to some particular design concept or to the entire repository system. Examples include both subsystem

1. The discussion of "modeling" in the text purposely focuses on the progressive modeling of *site-characterization data*, from the level of direct physical measurements to the overall performance of the entire repository system and its various components. On a separate logical plane, there is another extremely important type of modeling conducted by the Yucca Mountain Project: that associated with experimental work of various types to understand relevant fundamental physical principles. The results of this latter type of modeling must also be incorporated into all three "levels" of site-characterization modeling, including that conducted by this Study. Without an understanding of the proper physical behavior, all modeling of actual site data is likely to be futile.

evaluations and total-system performance assessment exercises.

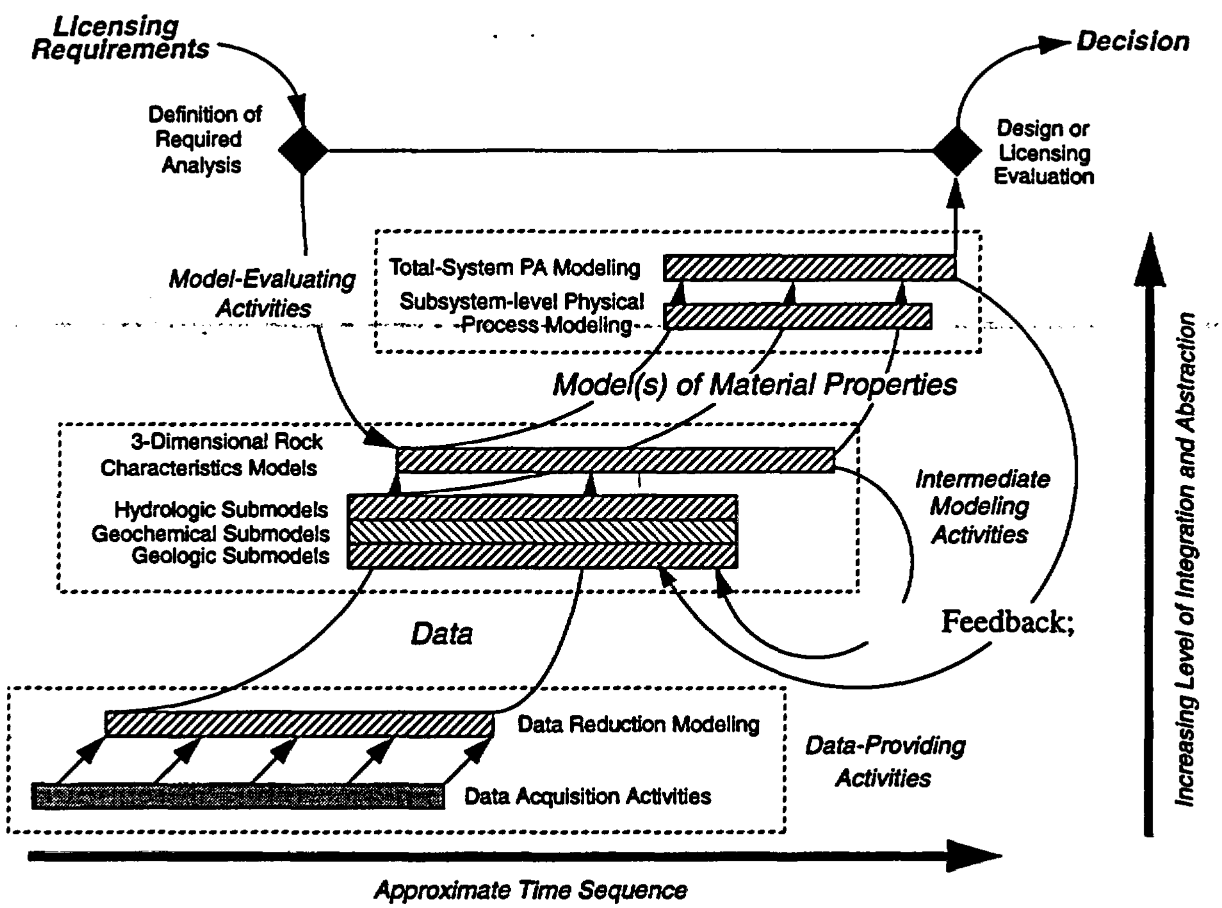

Figure 2.5 Conceptual representation of the relationship between various Yucca Mountain Project modeling activities, as driven by the need to conduct a particular design-evaluation or licensing analysis in order to arrive at a construction or licensing decision. Relationship is shown in the context of lower-level data-providing activities and higher-level model-evaluating activities (see discussion in text). Activities and models increase in degree of data integration and level of physical-process abstraction from top to bottom of diagram. Logical and approximate time sequence is from left to right (not to any particular scale).

The Three-Dimensional Rock Characteristics Models Study is in an intermediate position similar to, but slightly higher along the integration/abstraction continuum than what have been described in various Yucca Mountain Project planning documents as quasi-independently developed geologic, geochemical, and hydrologic submodels. The underlying data (physical properties measurements, geologic information, etc.) flow to the Three-Dimensional Rock Characteristics Models Study *through*, and *with benefit of understanding* developed by, the appropriate submodeling activity. On a mechanical level, the numeric material-properties data may be entered directly into a three-dimensional rock characteristics model produced by this Study, but the *context* of the more detailed understanding of the data is captured as well.[1] The output of the various geologic, geochemical, and hydrologic submodeling activities flows to high-level, summary, performance-assessment modeling *through* the activities of the Three-Dimensional Rock Characteristics Models Study, *which are specifically focused on the requirements* of the particular design-evaluation or performance-assessment analysis at hand (see Section 1.1). The integration and abstraction provided in the step from the several submodels to the three-dimensional rock characteristics model must be conducted in such a way that the significant geologic or hydrologic features of the site are captured *and* the resulting model is computationally tractable in the physical-process modeling exercise which follows. Iterative rock-characteristics modeling, combining interaction with both higher-level and lower-level modeling activities, may be required to pose the analysis properly (not shown on diagram, but see also Figure 2.4).

2.5 Tests Against Data and Similar Models

Testing any model against a similar type of model that has been developed independently is essentially a form of validation.[1] The relationship of this Study to similar intermediate-level modeling activities has been discussed previously in Section 2.4.3. As will be discussed later in this section (Section 2.5.4), comparison of the results of modeling conducted under this Study with the results of modeling conducted under the various studies described in Section 2.4.3 will serve as one form of model validation. In addition, because of the unique, detailed nature of the models to be produced under this Study, there are several other approaches to the validation of rock characteristics models. As described below, these approaches fall into three major categories: internal consistency including consistency with known data, comparison of alternative modeling methods, and favorable experience in predicting field results.

2.5.1 Internal Consistency

A model which is not consistent with itself or with known information obviously cannot be validated, except, perhaps for specific limited purposes directly related to the inconsistencies. Thus, a necessary, although not necessarily sufficient, condition for model validation is internal consistency. Internal consistency here is taken to imply consistency with objective site data that have been incorporated into the model in a meaningful manner.

2.5.1.1 Geometric Consistency

In some cases, the modeling method employed may ensure a certain degree of internal consistency. This aspect of validation becomes particularly important with respect to three-dimensional geometry. It is possible in manual model construction to develop a set of cross sections that appear reasonable geologically and that are "correct" in terms of the data portrayed on the section. However, such geologically reasonable cross sections may represent physical impossibilities in three dimensions. Manual validation of consistency typically consists of creating complementary long sections and cross sections that form an interlocking grid. If the individual geologic units portrayed on the set of sections can be traced around the grid in a consistent manner to the origi-

1. The understanding of fundamental physical principles developed by the type of modeling described in the footnote on page 36 is incorporated in this manner. This link is not shown on Figure 2.5 for the sake of simplicity.
1. It is recognized that some sources distinguish between "verification" and "validation;" however, there appears to be continuing disagreement as to exactly what is meant by each term. In this section, we use "validation" to convey the sense of testing a model against the underlying reality which that model is attempting to represent in simplified and/or numerical form.

nation point of a test case, the model can be judged to be internally consistent with respect to geometry. Such manual validation may be exceedingly labor intensive, and it is limited by the spatial distribution and reliability of the data.

Most computerized three-dimensional modeling packages include provisions for preventing logical inconsistencies associated with impossible three-dimensional geometry. Volume-oriented packages may have advantages over surface-modeling approaches (Section 2.2.1) in that generally the software simply will not allow the creation of overlapping volumes. A simplistic surface-modeling approach may not prevent the crossing of surfaces in space, which can lead to logical inconsistencies with respect to principles of stratigraphic superposition.

2.5.1.2 Statistical Consistency

Moving beyond (relatively) simple geometric considerations, there are several statistical approaches that may be applied to judge the validity of material properties models. Use of these techniques is particularly important in the case of simulated models, because these models are essentially the products of (sophisticated) random-number generators. Without a statistical sanity check, the old computer adage of "garbage in, garbage out" may be especially relevant.

Fortunately, the very nature of a numerical model may be used to confirm its validity. A conditional simulation should reproduce the input measured data if the model is sampled at the original data locations. If it is impossible to replicate exactly in the model the locations of samples in the real world (for example, some techniques relocate measured values to the nearest grid node for computational efficiency), checking the model at appropriate locations should yield values of the variable that are very close to the actual sample data. In similar manner, the univariate statistical measures (mean, variance, etc.) of the overall model should reproduce the statistics of the sample data set or they should vary away from those associated with the sample data in a manner that is in accordance with the modeling process used. For instance, interpolation algorithms, including kriging and other inverse-distance weighting schemes, are known to smooth out extreme values. Finally, if spatial continuity patterns have been incorporated into the models of material properties, the patterns observed in the completed models should be consistent with that of the data, again to the extent expected for the modeling technique employed.

2.5.2 Comparison with Alternative Modeling Approaches

Both geometric and material-properties models may be partially validated through comparison with equivalent models developed using an alternative modeling approach. The ultimate "alternative modeling approach," of course, is formal peer review. Given the complicated nature of material-properties models in particular, peer review may be the method of model validation generally employed to validate models constructed by this Study. Evaluation of internal consistency (Section 2.5.1) may be a component considered during peer review.

Other, more objective comparisons may also enter into a peer review, or simply form part of the general validation checking applied internally within this Study as part of the development and release of a particular model. For example, a few selected cross or long sections might be constructed manually and compared with equivalent sections extracted from a more comprehensive computer-generated model. Alternatively, a more-simplistic numerical modeling technique such as inverse-distance squared (Section 2.2.2.1) might be generated quickly and compared with a more sophisticated kriged or simulated model to see if the same general trends in property variability were being captured by both techniques.

2.5.3 Successful Predictive Experience

A major means of validating a numerical model of any type is successful use of the model in predicting a particular physical phenomenon. Geometric models may be used to predict the expected depth of a particular geologic contact in a new drill hole (or of a drill hole that was not used in the construction of the model (e.g., USGS, 1993). Models of material properties similarly can be used to predict values of a variable to be encountered at a particular location. Uncertainty measures may be incorporated either explicitly or after-the-fact through professional judgement.

2.5.4 Compatibility with Independently Developed Models

This means of model validation is essentially a variant of the approach described above in Section 2.5.2. However, in this case, the development of the model used for comparison would be essentially independent of this Study. The distinction is that the comparison is against a more-or-less completely separate interpretation of the objective data, which may or may not be directed toward similar goals. Additional discussion of the source of such independent models is given in Section 2.4.3.

2.5.5 Comparison Against Field-Scale Test Results

An approach to model validation, which is a conceptual combination of that described in both Section 2.5.3 ("Successful Predictive Experience") and Section 2.5.4 ("Compatibility with Independently Developed Models"), is the comparison of the models created as part of this Study Plan against the results of field-scale testing. This comparison and validation presumably could take place in either (or both) of two distinctly separate ways.

First, whereas the "successful predictive experience" of Section 2.5.3 is envisioned as applying to the prediction of values via a rock-characteristics model at essentially identical scales, this form of comparison/validation would involve the prediction of the larger-scale, block-effective material property actually measured by the field test. Successful validation of rock-characteristics models in this manner would lend a great deal of credibility to the modeling process and to the state of understanding of the physical system. The down-side of this type of comparison is that successful prediction involves at least two separate modeling processes; failure of either may result in a failure to predict accurately. (1) Rock characteristics modeling must be able to predict accurately the actual small-scale values (equivalent to the input data) existing (or likely to exist) at the location of the actual field test. (2) The techniques applied to scale up the small-scale input data must yield reasonable block-effective material properties. Although the up-scaling process is relatively simple for some material properties (see Section 2.2.2.4), scaling relationships for other properties are only poorly known. If the rock characteristics modeling process conducted under this Study can be "validated" through successful prediction of small-scale values (Section 2.5.3) measured as part of the large-scale field test and through successful up-scaling of basic, linear-averaging, framework properties, such as porosity or density, then perhaps an associated model based on small-scale measurements of less-successfully up-scaled (non-linear averaging) properties can be judged "validated" as well. It would remain to resolve the scaling issue; however, the scope of scaling in general is beyond this one Study Plan.

Second, this type of comparison/validation could focus on the *consequences* of the rock-characteristics models, rather than simply on the values of those models. As such, this approach is a variant of that described in Section 2.5.4, in that the comparison is against two independently developed "values" for some physical-process performance measure. This is in contrast to the simple comparison of two independently developed material-property models. Successful comparison of performance consequences would provide strong confirmation of the Project's description and understanding of at least a limited portion of the entire physical system. Again, however, "failure" of the comparison does not necessarily invalidate the rock characteristics modeling portion of the work, because modeling of a physical-process — which is beyond the scope of this Study Plan — is also involved.

Specific details of how this type of validation exercise might be implemented are impossible to specify in this Study Plan. It is presumed that many, if not all, SCP activities proposing field-scale testing will incorporate a similar type of comparison of observe physical-process results with predicted processes based on material property measurements collected as part of those activities. Thus, to some extent, this entire type of comparison may be judged to be beyond the scope of this Study. This discussion does, however, accentuate the need emphasized throughout this Study Plan of close interaction of various Project participants involved in site characterization, integration of data, and modeling of physical processes (Sections 2.4, 3.0).

2.6 Incorporation of New Data

2.6.1 Updating of Models

Details of how (and if) new data from site characterization are incorporated into the rock characteristics models created under this Study are dependent upon the specific model under consideration and the circumstances and techniques associated with that model. In many cases, new data simply will not be incorporated, *per se*, into a particular model because the purposes served by that model are likely to have already been accomplished. This is in general accordance with the *ad hoc* nature of the modeling conducted by this Study. Thus, a principal means of incorporating new data will be the construction of completely new models.

Geometric models are a probable exception to the previous statement. Because geometric models form an overall framework into which a variety of material properties models can be fitted, it is more likely that the framework will need to be built up over a substantial time period and thus need to be updated episodically with the results of new site characterization activities.

The mechanics of such updating depend upon the modeling methodology. In some instances and depending upon the specifics of the new data to be incorporated, effectively the entire model may need to be recreated. In other instances, the changes may be effected simply by mapping the new data into the proper model location(s) and adjusting stratigraphic boundaries or other model entities to accommodate the now-known information.

An important corollary of the fact that new site characterization data will be obtained even as modeling is ongoing, and thus leading to the need for episodic updating, is that the new information will provide an important opportunity to validate the earlier models, the modeling technique, and any associated uncertainty measures. Successful predictive experience as a means of model validation has been discussed in Section 2.5.3.

2.6.2 Consequence Evaluation

Because of the direct tie between this Study and the end users of the rock characteristics models created hereunder, there is a feedback loop established (Figure 2.4) that bears on issues of data adequacy and the impact of new data on previously constructed models. The rock characteristics models of this Study are generally created for a specific purpose in design evaluation or performance assessment. If new data become available, the end-user evaluation activity may well request that the input material properties model(s) be revised so that the analysis may be re-examined. If the *consequences* of the evaluation do not change materially, this stability may be an indication that the body of site characterization information is now adequate, and that there is little to be gained by continuing site investigations *for these purposes.*

Some of the modeling techniques internal to the Three-Dimensional Rock Characteristics Study may serve much the same purpose. For example, post-processing techniques, such as described in Section 2.2.2.2, under *Geostatistical Simulation*, can produce maps showing the probability of obtaining various levels of a particular variable. Incorporation of new data into a set of simulations may not materially alter such a probability map. If this is the case, the data may be judged adequate, even without processing the revised models completely through an end-user physical-process model.

3.0 APPLICATION OF RESULTS

Because the Three-Dimensional Rock Characteristics Study develops most of its models in response to requests by specific other Yucca Mountain Project activities, the most direct application of the models will be in those requesting studies or activities. In a broader, more programmatic context, there are three principal areas of application, in addition to final preparation of licensing documents. These areas are as feedback to site characterization, development and evaluation of various design alternatives, and performance assessment.

3.1 Feedback to Site Characterization

The position of the Three-Dimensional Rock Characteristics Models Study in an intermediate position between data-generating site characterization activities and process-evaluating design and performance-assessment activities (Figure 2.5) places it in a unique position with respect to providing feedback to site characterization regarding issues of data adequacy. This feedback mechanism was discussed previously in Sections 2.4 and 2.6.2. Feedback would be directed to the appropriate study(ies) indicated in Tables 2.5 and 2.6. It is important to note that it is the *consequences of uncertainty* that are the primary focus in evaluating data adequacy. Even though the uncertainty in interpretation or in the resulting rock characteristics models may be scientifically intriguing; to the extent that the particular design, performance assessment, or licensing decision under consideration is insensitive to that uncertainty;, the data are adequate for their purpose.

In a more proactive role, modeling activities conducted under this Study may be able to identify regions within the site area that exhibit greater variability or uncertainty, or which appear to be the location of spatially inconsistent information. Apparently inconsistent geometric information regarding stratigraphic contacts or unit thicknesses may be suggesting the presence of heretofore unsuspected faulting or stratigraphic changes, and thus indicate a need for additional site characterization information in particular regions or geologic intervals. Evaluation of a set of equally likely geostatistical simulations may indicate major variability in certain portions of a modeled volume. Rautman and Robey (1994) produced quantitative summaries of contact uncertainty for selected geologic contacts as part of the Total-System Performance Assessment modeling exercise for 1993.

3.2 Design Development and Evaluation

The models developed by the Three-Dimensional Rock Characteristics Models Study will be used in two principal roles during the development and evaluation of engineering designs related to the Exploratory Studies Facility and potential repository. The first role deals mostly with the location of various proposed engineered structures. Models of the three-dimensional position of appropriate engineering units in space are required to ensure that facilities are excavated in the proper physical and geologic position. Avoiding (or purposely encountering) fault zones, regions of dense fracturing, or materials of a particular rock type requires a spatial representation of where those features are likely to be located. Evaluation of design alternatives that may focus on potential expansions of the waste-storage area(s) or alternative drift configurations within the underground facility will draw heavily on the geometric aspects of the three-dimensional rock characteristics models produced by this Study.

A second, and arguably more unique and significant, application of the models developed by this Study focuses on evaluating the performance of various engineered features. Although the geometry of the model is definitely of importance, the quantitative evaluation of engineering designs most likely will focus on the distributions of material properties in space, created as described in Section 2.2.2. Some of the design-related analyses that are anticipated include evaluation of drift stability under in-situ conditions and in reaction to stresses induced by thermal loading from the waste packages (a function of mineral composition and other factors; related to preclosure safety and to retrievability), changes in fracture patterns induced by thermal loading (which may affect ground-water flow), dry-out of the rock mass caused by mine ventilation, and thermal uplift of the ground surface.

Although the distinction between design-evaluation analyses and short-term performance assessment (see Section 3.3) is somewhat arbitrary, we assume that "design evaluations" probably will involve more local detail, such as may be captured through geostatistical simulation, and will be more sensitive to local heterogeneities than larger-scale "performance assessments," particularly those cast in the total-system performance framework. Accurately quantifying the uncertainty associated with the description of the rock mass may allow engineers to establish a factor of safety for the particular system being designed. Potentially, better quantitative understanding of geologic uncertainty could allow a smaller factor of safety to be used in design, leading to reduced the costs of construction.

A listing of the design-evaluation activities believed to be relevant to the Three-Dimensional Rock Characteristics Models Study is presented in Table 3.1.

Table 3.1 Partial List of Design-Evaluation Activities Relevant to the Three-Dimensional Rock Characteristics Models Study, Developed from the SCP

SCP Section	Related Information Need	Brief Description	Tie to This Study
8.3.2.2.1	1.11.1	Site information needed for design	Specific request for reference stratigraphic geometry and thermomechanical rock properties (SCP Table 8.3.2.2-5)
8.3.2.2.3	1.11.3	Design concepts for orientation, geometry, layout, and depth of the underground facility	Specific request for site geologic data describing system geometry
8.3.2.2.5.2	1.11.5	Analyses of drift and pillar stability to limit excavation-induced changes in rock permeability	Same as SCP Section 8.3.2.2.1
8.3.2.2.6	1.11.6	Repository thermal loading and predicted thermal and thermomechanical response of the host rock	Same as SCP Section 8.3.2.2.1

Table 3.1 Partial List of Design-Evaluation Activities Relevant to the Three-Dimensional Rock Characteristics Models Study, Developed from the SCP

SCP Section	Related Information Need	Brief Description	Tie to This Study
8.3.2.4.1.1	4.2.1	Analyses needed to design ramps and drifts, including ground support; establish the locations of the disposal horizon, develop safe construction techniques, design and evaluate effects of the ventilation system.	Specific request for system geometry, rock water content, and thermal conductivity; also reference to SCP Section 8.3.2.5.7
8.3.2.5.1	4.4.1	Site and performance assessment information needed for design	Specific request for system geometry and material properties (SCP Table 8.3.2.5-2)
8.3.2.5.7	4.4.7	Design analyses addressing impacts of surface conditions, rock characteristics, hydrology, and tectonic activity	Specific request for models of site geometry, rock properties
8.3.3.2.1	1.12.1	Site, waste package, and underground facility information needed for design of seals	Specific request for material properties at the locations of proposed seals
8.3.5.2.1	2.4.1	Site and design data needed to support retrieval	Same as SCP Section 8.3.2.5.1

3.3 Performance Assessment

3.3.1 Preclosure Performance Assessment

Licensing regulations specify a number of requirements related to the preclosure performance of a potential repository (10 CFR 60.131-134). Although closely related to the engineering design evaluations discussed in Section 3.2, these preclosure performance analyses probably will emphasize the time period through mandated retrievability of the waste and the effects of thermal loading to a greater extent than simple design evaluations focused on constructability.

3.3.2 Postclosure Performance Assessment

A very significant use of the models produced by the Three-Dimensional Rock Characteristics Study is to resolve postclosure performance issues related to the two "geologic," or "site-oriented," regulatory licensing criteria: (1) the pre-waste-emplacement ground-water travel time requirement, and (2) the total-system radionuclide release requirements. These are Issues 1.6 and 1.1 (respectively) in Table 1.1. Resolution of these and most of the other issues listed in the table depend upon a comprehensive, modeled interpretation of the site based upon limited physical description. Additionally, although the guidelines for nuclear waste repositories of 10 CFR 960 are formally no longer relevant in terms of site selection (see description of the siting process contained in 10 CFR 960.3-2) because the Yucca Mountain site has already been "selected" for site characterization, the Department of Energy is continuing to evaluate the Yucca Mountain site for suitability in terms of the "disqualifying conditions" contained in the regulations. Prominent among the ongoing considerations relevant to future evaluations of site suitability at Yucca Mountain is the ground-water travel time specification (10 CFR 960.4-2-1(d)) that forms the basis for Issue 1.6.

3.3.2.1 Ground-Water Travel Time Issue

Understanding the ground water flow system as it currently exists is one of the foremost requirements of performance assessment. Site characterization will acquire data on infiltration and potential recharge rates as a function of spatial position on the mountain. Significant variation in precipitation has been reported (Hevesi et al., 1992). How this moisture is redistributed in the near-surface environment, including partitioning into vertically downward and laterally diverted flow components will require modeling. Numerical models of the relevant material properties will be required to understand the effective recharge/flux affecting Yucca Mountain. Understanding deep percolation of ground-water in the unsaturated zone will also require numerical process modeling. This modeling also requires numerical models of rock characteristics, such as those produced by this Study. Finally, a major component of the modern-day flow system is within the saturated zone below the potential repository level (Winograd and Thordarson, 1975; Czarnecki and Waddell, 1984). Much of this flow is widely assumed to be occurring independent of the immediately overlying unsaturated flow system (e.g., Czarnecki and Waddel, 1984; Montezar and Wilson, 1984), although understanding the coupling between local downward fluxes and laterally moving through fluxes of the regional ground-water system will be important.

3.3.2.2 Cumulative Radionuclide Releases

Somewhat separate from the issue of the currently existing, pre-waste-emplacement flow system is the issue of radionuclide transport away from emplaced waste. The advective transport of contaminants escaping from waste packages may be approximated by the current ground water flow system. However, the presence of zeolites along potential flow paths will allow sorption and retardation of radionuclides. For example, there is a profound change in the distribution of zeolitic minerals from north (near drill hole USW G-1), where certain stratigraphic intervals are wholly zeolitic (Spengler, et al., 1981), to south (USW G-3), where the same intervals are entirely vitric (Scott and Castellanos, 1984). Three-dimensional models of zeolite distribution (similar to that of Ortiz and others, 1984), including the spatially varying distribution of compositional variants within this broad class of minerals (e.g., Bish and Vaniman, 1985), may be particularly important in determining total radionuclide releases at the accessible environment. Uncertainty issues regarding the effectiveness of such retardation may play a prominent role in licensing arguments. The interaction of rock matrix with through-going fractures similarly may affect radionuclide transport. Three-dimensional models of the distribution of fractures of varying aperture and mineral coatings may be important input to numerical process modeling conducted in support of postclosure performance assessment.

Postclosure performance assessment will also focus on changes induced in the pre-existing natural system by the physical presence of the waste and constructed repository. Scenarios have been constructed related to thermally driven convection cells that may concentrate *in-situ* moisture into a condensate "cap," which later may collapse back upon the waste packages as the heat generated by the waste decays (e.g., Buscheck and Nitao, 1993). The existence of heterogeneous hydrologic properties may significantly affect the development of such convective cells and/or the final dissipation of the water. Detailed representations of spatially variable material properties almost certainly will be required to address the existence and extent of phenomena such as this. Once the detailed local behavior of the thermally stressed hydrologic system is understood, it will then be necessary to simplify this, and other processes, for use in modeling the performance of the total repository system. A simplified, one-dimensional example of the application of the stochastic-simulation approach to performance assessment modeling as applied to Yucca Mountain, in which descriptive rock characteristics models are coupled to a hydrologic flow model, has been presented by Rautman and Treadway (1991).

A listing of the major performance assessment-related activities relevant to the Three-Dimensional Rock Characteristics Models Study is presented in Table 3.2. A short listing of

Table 3.2 Partial List of Performance Assessment Activities Relevant to the Three-Dimensional Rock Characteristics Models Study, Developed from the SCP

SCP Section	Related Information Need	Brief Description	Tie to This Study
8.3.5.12.1	1.6.1	Site information needed to identify the fastest path of likely radionuclide travel and to compute ground-water travel time along that path	Specific request for (a) system geometry and (b) material property values
8.3.5.12.2	1.6.2	Calculational models needed to predict ground-water travel time	Specific request for three-dimensional model of material properties
8.3.5.12.3	1.6.3	Identification of paths of likely radionuclide travel from the disturbed zone to the accessible environment and identification of the fastest path	Restatement of Information Needs 1.6.1 (SCP Section 8.3.5.12.1) and 1.6.2 (SCP Section 8.3.5.12.2.)
8.3.5.12.4	1.6.4	Determination of pre-waste-emplacement ground water travel time along the fastest path of likely radionuclide travel from the disturbed zone to the accessible environment	Restatement of Information Needs 1.6.1 (SCP Section 8.3.5.12.1), 1.6.2 (SCP Section 8.3.5.12.2.), and 1.6.3 (SCP Section 8.3.5.1.2.3)
8.3.5.12.5.1	1.6.5	Ground water travel time after repository construction and waste emplacement	Post-construction version of SCP Section 8.3.5.12.4; specific request for system geometry and material properties (SCP Table 8.3.5.12-5)
8.3.5.13.1	1.1.1	Site information needed to calculate releases to the accessible environment	Specific request for material properties and system geometry (SCP Table 8.3.5.13-17)
8.3.5.13.3	1.1.3	Calculational models for predicting releases to the accessible environment attending realization of potentially significant release-scenario classes	Same properties and models as in SCP Section 8.3.5.12.1, and including properties for overburden rock units

Table 3.2 Partial List of Performance Assessment Activities Relevant to the Three-Dimensional Rock Characteristics Models Study, Developed from the SCP

SCP Section	Related Information Need	Brief Description	Tie to This Study
8.3.5.13.4	1.1.4	Determination of radionuclide releases to the accessible environment associated with realizations of potentially significant release scenario classes	Same as above
8.3.5.13.4.2	1.1.4	Provision of simplified, computationally efficient models of the final scenario classes representing the significant processes and events from 10CFR60.112 and 60.115	Same as above; developing simplified models implies a coherent understanding of underlying complex models
8.3.5.13.5	1.1.5	Probabilistic estimates of radionuclide releases to the accessible environment considering all significant release scenarios.	Specific request for material properties and system geometry (SCP Table 8.3.5.13-17)
8.3.5.14.1.1	1.2.1	Calculation of doses to the public through the ground water pathway	Same as SCP Section 8.3.5.13.4
8.3.5.14.2.1	1.2.2	Calculation of transport of gaseous carbon-14 dioxide through the overburden	Same as SCP Section 8.3.5.13.3
8.3.5.14.2.2	1.2.2	Calculation of doses to the public through the gaseous pathway of carbon-14	Same as above

related modeling that is conducted under various site characterization studies is presented in Table 3.3.

Table 3.3 Other Modeling Studies Described in the SCP

SCP Study	Title
8.3.1.2.1.4	Regional Hydrologic System Synthesis and Modeling
8.3.1.2.2.9	Site Unsaturated Zone Modeling and Synthesis
8.3.1.2.3.3	Saturated Zone Hydrologic System Synthesis and Modeling
8.3.1.3.2.1	Mineralogy, Petrology, and Chemistry of Transport Pathways
8.3.1.3.7.1	Retardation Sensitivity Analysis
8.3.1.4.2.3	Three-Dimensional Geologic Model

Table 3.3 Other Modeling Studies Described in the SCP

SCP Study	Title
8.3.4.2.4.1	Characterize Chemical and Mineralogical Changes in the Post-emplacement Environment
8.3.4.2.4.2	Hydrologic Properties of Waste Package Environment
8.3.4.2.4.3	Mechanical Attributes of the Waste Package Environment

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4.0 SCHEDULE AND MILESTONES

4.1 Beginning and Ending Dates

The creation of preliminary three-dimensional rock characteristics models to develop and refine modeling techniques and to demonstrate the significance of the uncertainty-assessment methods that will play an important role in this Study has been on-going for some time (e.g., Rautman, 1990; Rautman and Treadway, 1991; Rautman and Robey, 1993, 1994). All of these preliminary models are judged "non-quality affecting" (non-QA). The production of quality-affecting models will commence upon approval of this Study Plan.

To a large extent, the modeling to be conducted under this Study will be complete when the License Application (LA) is completed and submitted to the Nuclear Regulatory Commission. However, it is probable that the Commission may question portions of the initial DOE license submittal and require clarification or expansions. Potentially, the Three-Dimensional Rock Characteristics Models Study will be required to conduct additional modeling to resolve these types of concerns. The role of this Study in post-License Application performance-confirmation activities has not yet been defined.

4.2 Milestones

Experience has shown that definition of detailed milestones and schedules associated with studies must be sufficiently flexible that it is difficult to state these with confidence in a high-level planning document such as a study plan. This is particularly true for the Three-Dimensional Rock Characteristics Models Study, which will produce a major portion of its products essentially on-demand for different end users in design evaluation and performance assessment. Specific milestones for deliverable rock characteristics models will be developed as part of on-going Project planning activities using PACS (Planning and Control System). These milestones and deliverables will be the result largely of negotiated agreements with potential customers of this Study, specifying the content and format of the resulting models of rock characteristics. Start and end dates would flow from the milestones and other requirements driving the end-user activity.

As a general philosophy, however, this Study is guided by the major Project-level milestones associated with (1) Advanced Conceptual Design (ACD) and (2) License Application Design (LAD). Although the licensing strategy being pursued by the Yucca Mountain Site Characterization Project continues to evolve, this strategy will, without question, involve a number of progressive milestones and "applications" from the U.S. Department of Energy to the U.S. Nuclear Regulatory Commission. Each of these major milestones will be associated with significant performance-assessment evaluations of site characterization data as it exists as of a certain "freeze" date. It is the intent of this study to conduct major modeling efforts in support of to-be-determined design evaluations and performance-assessment activities that are (or will be) linked to the ACD and LAD (potentially to be renamed) data freezes and other deliverable products. The specific milestones and modeling products to be generated by this study will be developed as Project planning associated with these milestones proceeds.

In addition, the Yucca Mountain Project has committed to a process of conducting major, interim performance assessment exercises at roughly two-year intervals (Figure 4.1) to demonstrate progress in (a) understanding the technical suitability of Yucca Mountain as a potential site for a repository and (b) developing the capability to conduct realistic performance-assessment calculations. These periodic performance assessments presumably are tied to interim evaluations of the suitability of the Yucca Mountain site for licensing. It is the intent of this Study to produce increasingly sophisticated material-properties modeling to support the various total-system performance assessment exercises as the scope of those exercises is determined.

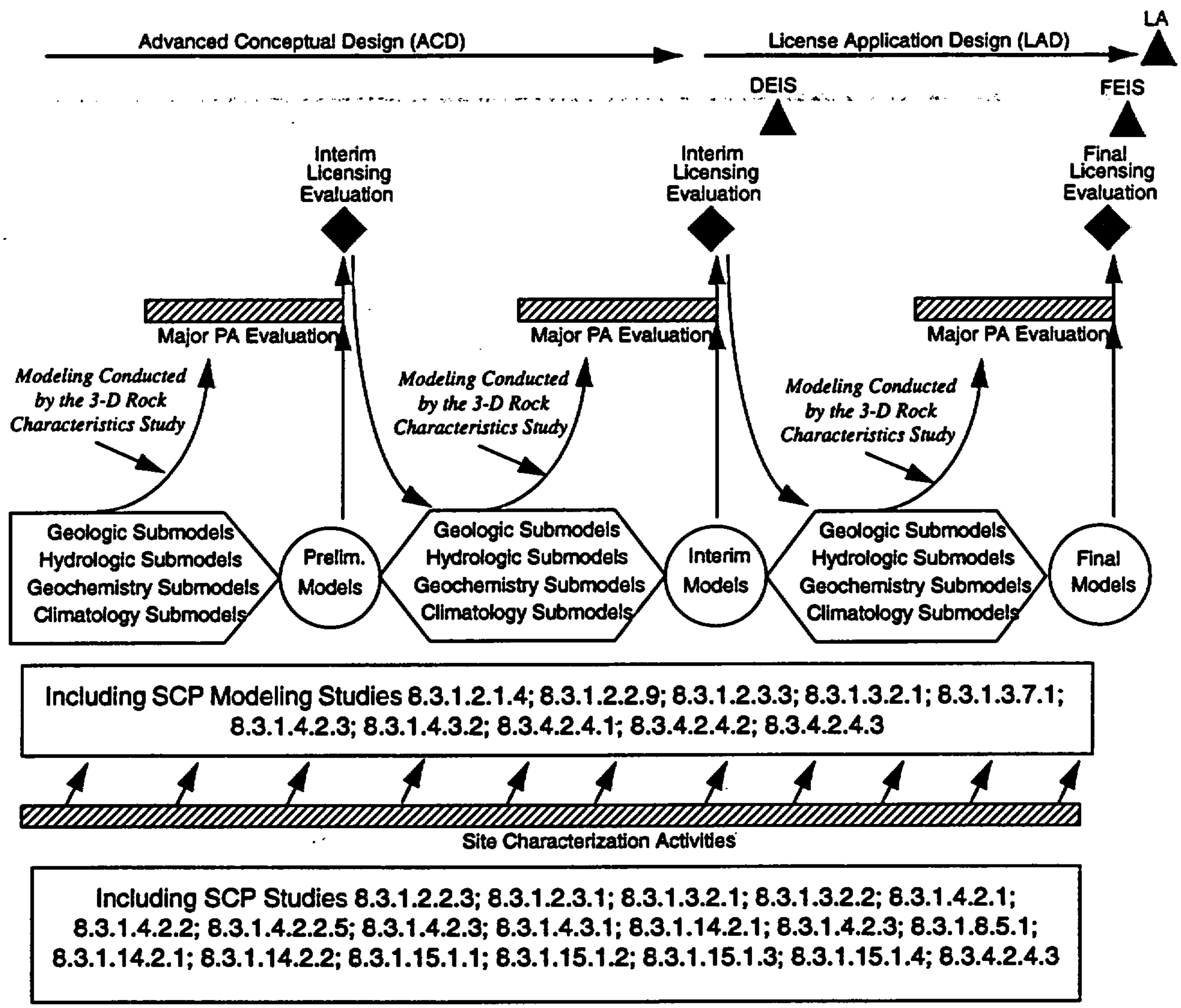

Figure 4.1 Schematic, conceptual schedule for completion of various modeling exercises and their relationship to some major evaluations of site suitability and licensing milestones. By reference to Figure 2.5, this Study is represented by the upward-sweeping arrows, integrating and simplifying the various indicated submodels to meet the specific requirements of the performance assessment evaluations. Time progresses from left to right, but is not to scale. The specific number of iterations has not been determined by the Project.

Separately from the issue of milestones related to major Project-level modeling activities and licensing decisions, there are a number of subactivities within this Study necessary to accomplish the larger-picture support to performance assessment and design. These are represented conceptually in Figure 4.2. As represented on the diagram, preliminary modeling activities have been underway for some time. These preliminary rock characteristics models have been used principally in various preliminary performance-assessment type activities (e.g., Wilson et al., 1994), and they have identified a number of software-development efforts that are required for efficient and traceable production of quality affecting models. Preliminary (non-QA) modeling will continue as appropriate to evaluate new modeling algorithms or approaches. Software-development efforts will continue throughout the period of activity by this Study in order to implement new or improved modeling techniques and algorithms. Development efforts will be most intense early in the Study, diminishing later on as an effective and adequate production environment is developed.

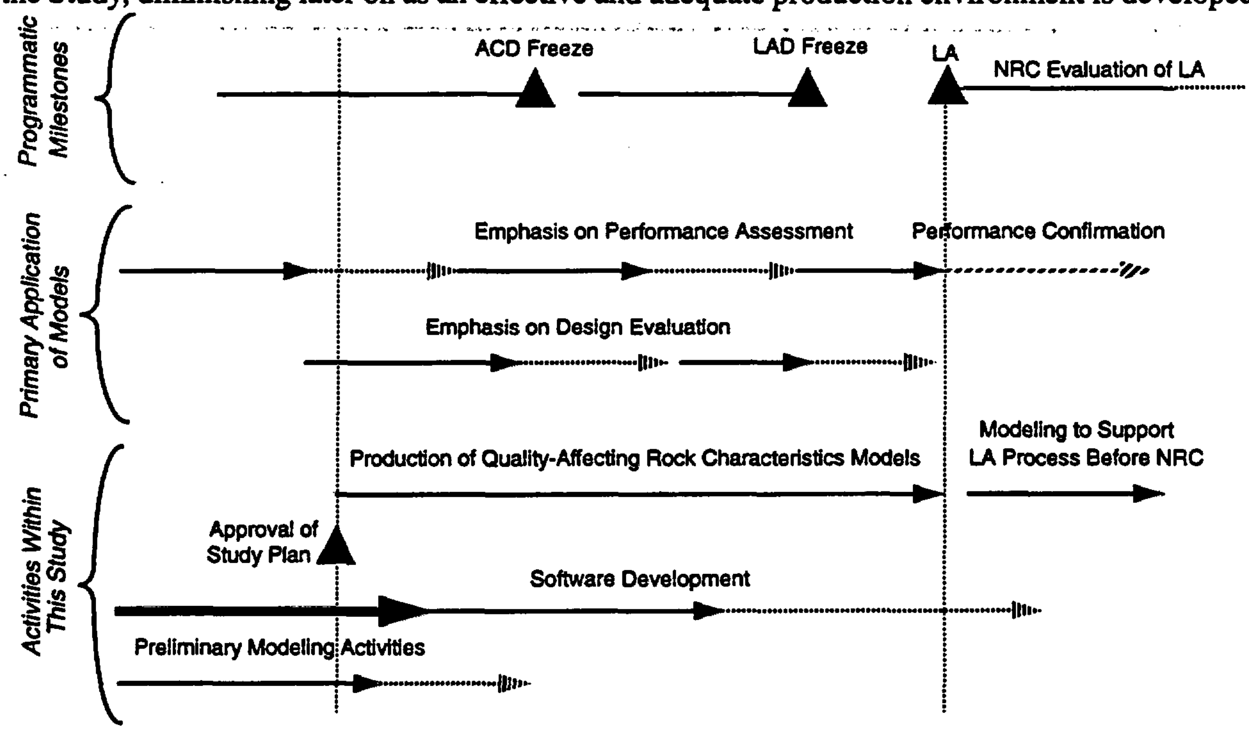

Figure 4.2 Schematic conceptualization of the relationships among some internal activities within this Study, the application of the resulting models, and the high-level programmatic milestones which drive the modeling. Diagram illustrates alternating (but non-exclusive) emphasis on design-evaluation modeling and performance-assessment modeling related to Project-level design milestones (Advanced Conceptual Design: ACD, and License Application Design: LAD). Time progresses from left to right, but is not to scale. Weight of arrows is intended to represent relative effort devoted to the specified activity. No specific data feeds are shown for simplicity; however, within this study, the state of knowledge proceeds generally upward across the indicated activities. The line labeled "Production of Quality-Affecting Rock Characteristics Models" is portrayed in expanded, but still schematic form in Figure 4.3.

Beginning with approval of this Study Plan, this Study will begin production of fully qualified, traceable models. It is anticipated that in the period leading up to completion of ACD, there will be increased emphasis on modeling to support various design-validation and evaluation activities. Once a "freeze" has been declared to the advanced conceptual design, rock characteristics modeling is anticipated to shift focus to activities that evaluate the performance consequences of that design in light of available site-characterization information. A similar change of emphasis is anticipated to be associated with development of the final license application design, followed by performance modeling of the LAD repository configuration. The relationship of these two types of modeling is not exclusive, nor are the resulting models incompatible with one another. The differences between the two principal types of models probably will reflect differences in scale appropriate to the use of the numerical model in further analysis (see discussion in Section 3.2 on page 43).

Performance-type modeling will almost certainly continue beyond the date of freezing the license-application design, and production of rock characteristics models will continue to support development of the license application (LA) itself. Figure 4.2 indicates that modeling under this study may continue after submission of the license application to the Nuclear Regulatory Commission as required to clarify any questions regarding suitability of the site or adequacy of the license application (Section 4.1). The exact nature and extent of this modeling support is poorly defined at present.

A schematic schedule of the types of detailed technical work activities involved in a specific rock-characteristics modeling exercise is presented in Figure 4.3. Again, although the specific work activities that will be needed to accomplish a specific rock characteristics modeling exercise will depend upon the specific type of modeling activity, a number of "generic" work activities can be identified *a priori*. The initiating event is the identification of the need for a specific type of material property model by a user, or customer, in the terminology of Figure 2.4. Interaction with the end-user of the rock-characteristics model(s) will lead to joint development of and agreement on the concept to be used in modeling rock characteristics (Figure 4.3). Relevant criteria include the extent of the model domain, the nature of discretizing or gridding that domain, the required input data and other information to be used in developing the model(s), and specification of the format in which the model(s) will ultimately be delivered. All of these criteria must be formulated in such a manner that the specific objective of the using design evaluation or performance assessment analysis will be accomplished.

Various types of exploratory data analysis (Figure 4.3) precede and overlap with the creation of initial, "prototype" models. Iterations between statistical analyses of data and preliminary modeling which attempts to capture the important "essence" of the actual geology, are not shown for sake of simplicity. The prototype model(s) may be transferred to the user for preliminary evaluation to ensure that the output format is, indeed, suitable for its intended use. Possible revisions of the modeling criteria are possible if, for example, the numerical process-modeling code cannot handle the internal variability of the numerical rock-characteristics model. A parallel activity to validate the model (see section 2.5) would be conducted internal to this Study. These activities collectively constitute the model development stage (Figure 4.3), which is probably the most time-consuming process, because of the need to "explore" and commit mistakes while coming to an appropriate level of understanding of the natural system and its numerical representation.

Once the user agrees that the material-property models and their numerical representation are acceptable, production of final models for actual use in design evaluation or performance

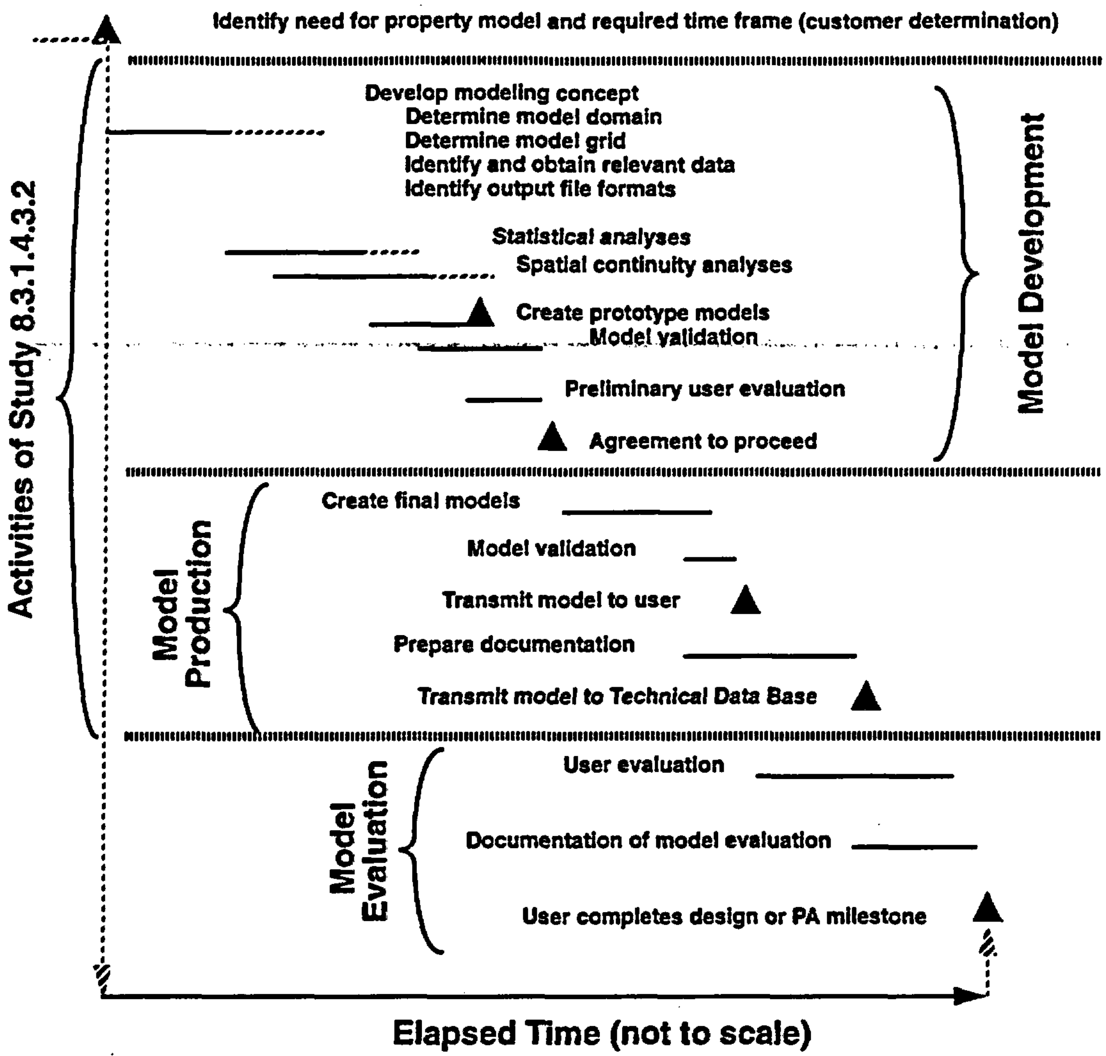

Figure 4.3 Conceptual flow diagram of work activities involved in creating a generic rock-characteristics model. Lines suggest the potential duration of various work activities; solid triangles represent discrete events, such as milestones and/or deliverable products

assessment can commence (Figure 4.3). The duration of this model production stage will be determined mainly by computational considerations. Generation of a suite of large, simulated models will require more computational time than the creation of an estimated model of similar physical size. The independence of individual stochastic realizations means that large simulation exercises could be accelerated through the use of distributed computing environments. Following some type of validation of these final models (or a subset), they (it) would be released to the user for use in the intended physical-process modeling exercise. Creation of documentation of the rock characteristics model (Figure 4.3) is shown extending in time both before and after delivery of the final product to the customer. Users require a certain amount of documentation to use a rock-properties model effectively; however, that documentation need not be in final, publication-quality form to be useful. The model production stage terminates with transmittal of the created model(s) to the Yucca Mountain Project technical data base for archiving and other use.

The model evaluation stage, shown in the lower portion of Figure 4.3, actually occurs outside the purview of this Study. This representation of the end-user's activities, which is very conceptual in nature, is included to suggest that the time required from start to finish of a design evaluation or performance assessment activity includes both the construction of three-dimensional rock characteristics models and the processing of those models through the necessary analytical or numerical codes. The absolute time from start to finish could be as short as a month of concentrated effort, or it might extend over a year or more in the case of a major total-system performance assessment.

4.3 Interrelationships and Data Dependencies with Other Studies

The Three-Dimensional Rock Characteristics Study is dependent upon many of the studies within the site characterization program (Section 2.4). Specifically, geologic and other input is required from the site drilling programs (Table 2.5). Without this fundamental input regarding the physical description of the Yucca Mountain site, quantitative modeling of the site is impossible. Additionally, because the Three-Dimensional Rock Characteristics Study particularly emphasizes the quantitative modeling of spatially varying physical properties, the Study is highly dependent upon the results of many of the laboratory testing studies, especially those described in Table 2.6. The numerical values of material properties are necessary to develop models of spatial continuity and to constrain the modeling algorithms to respect what is known about the Yucca Mountain site.

Additional detail regarding the interrelationship of the Three-Dimensional Rock Characteristics Study with other site characterization studies is presented in Sections 2.4, 2.5, and 3.0. A conceptual, but instructive diagram showing the relationship of this Study to both site characterization studies and to a number of (implied) modeling activities within the Yucca Mountain Project is presented in Figure 2.5.

5.0 REFERENCES

Almeida, A.S., 1993, Joint simulation of multiple variables with a Markov-type coregionalization model, in: *Report 6*, May 1993, Stanford Center for Reservoir Forecasting, Stanford University.

Anderson, M.P. and W.W. Woessner, 1992, Applied groundwater modeling, San Diego: Academic Press. Inc., 381 p.

Bish, D.L., and D.T. Vaniman, 1985, Mineralogic summary of Yucca Mountain, Nevada: Los Alamos Report LA-10543-MS, Los Alamos National Laboratory, Los Alamos, N. Mex., 55 p.

Boyd, P.J., R.J. Martin III, and R.H. Price, 1994, An experimental comparison of laboratory techniques in determination of bulk properties of tuffaceous rocks: *Sandia Report SAND92-0119*, Sandia National Laboratories, Albuquerque, New Mexico, 46 p.

Buscheck, T.A, and J.J. Nitao, 1993, Repository-heat-driven hydrothermal flow at Yucca Mountain, Part I: Modeling and analysis: *Nuclear Technology*, v. 104, p. 418-448.

Bush, D., and R.E. Jenkins, 1970, Proper hydration of clays for rock property determination: *Journal of Petroleum Technology*, p. 800-804.

Clark, I., 1979, Practical Geostatistics, New York: Elsevier Applied Science Publishers, 129 p.

Czarnecki, J.B., and R.K. Waddell, 1984, Finite-element simulation of ground-water flow in the vicinity of Yucca Mountain, Nevada-California: *U.S. Geol. Surv. Water-Resources Investigations. Report 84-4349*, 38 p.

David, M., 1977, *Geostatistical ore reserve estimation*, Developments in Geomathematics 2, New York: Elsevier Scientific Publishing Company, 364 p.

Davis, J.C., 1986, Statistics and data analysis in geology, New York: John Wiley and Sons, 646 p.

Desbarats, A.J., 1987, Numerical estimation of effective permeability in sand-shale formations: *Water Resources Research*, v. 23, p. 273-286.

Desbarats, A.J., and R. Dimitrakopoulos, 1990, Geostatistical modeling of transmissibility for 2D reservoir studies: SPEFE (Dec. 1990), p. 437-443.

Deutsch, C., 1987, Calculating effective absolute permeability in sandstone/shale sequences: *Soc. Petrol. Eng. Paper 17246.*

Deutsch, C.V. and A.G. Journel, 1992, *GSLIB Geostatistical subroutine library and user's guide*, New York: Oxford University Press, 340 p.

DOE (U.S. Department of Energy), 1988, Site characterization plan, Yucca Mountain site, Nevada Research and Development Area, Nevada: *Report DOE/RW-0199*, U.S. Department of Energy, Office of Civilian Radioactive Waste Management.

Dudley, A.L., R.R. Peters, J H. Gauthier, M.L. Wilson, M.S. Tierney, and E.A. Klavetter, 1988, Total System Performance Assessment Code (TOSPAC) Volume 1: Physical and Mathematical Bases, *Sandia Report SAND85-0002*, Sandia National Laboratories, Albuquerque, New Mexico.

Hevesi, J.A., A.L. Flint, and J.D. Istok, 1992, Precipitation estimation in mountainous terrain using multivariate geostatistics. Part II: Isohyetal maps: *Journal of Applied Meteorology*, v. 31, p. 677-688.

Gomez-Hernandez, J.J., 1992, Direct stochastic modeling of block effective absolute permeability: A geostatistical approach, Stanford, CA: Stanford (University) Center for Reservoir Forecasting, *Report 5*.

Isaaks, E,H., 1990, The application of Monte Carlo methods to the analysis of spatially correlated data: Ph.D. thesis, Stanford University, Stanford, Calif.

Isaaks, E.H., and R.M. Srivastava, 1989, *An introduction to applied geostatistics*, New York: Oxford University Press, 561 p.

Istok, J.D., C.A. Rautman, L.E. Flint, and A.L. Flint, 1994, Spatial variability in hydrologic properties of a volcanic tuff: *Ground Water*, v. 32, p. 751- 760.

Iman, R.L., and M.J. Shortencarier, 1984, A FORTRAN 77 program and user's guide for the generation of Latin hypercube and random samples for use with computer models: *Sandia Report SAND83-2465*, Sandia National Laboratories, Albuquerque, New Mexico, 50 p.

Jensen, J.L., 1991, Use of the geometric average for effective permeability estimation: *Mathematical Geology*, v. 23, p. 833.

Journel, A.G., 1983, Nonparametric estimation of spatial distributions: *Mathematical Geology*, v. 15, p. 445-468.

Journel, A.G., 1989, Fundamentals of geostatistics in five lessons, Washington DC: Am. Geoph. Union, *Short course in geology*, v. 8, 40 p.

Journel, A.G., and F. Alabert, 1989, Non-gaussian data expansion in the earth sciences: *Terra Nova*, v. 1, p. 123-134.

Journel, A.G., C. Deutsch, and A.J. Desbarats, 1986, Power averaging for block effective permeability: *Soc. Petrol. Eng. Paper 15128*.

Journel, A. G., and J. J. Gomez-Hernandez, 1989, Stochastic imaging of the Wilmington clastic sequence: *SPE Reprint 19857*, Soc. Petrol. Engineers.

Journel, A.G., and Ch.J. Huijbregts, 1978, *Mining geostatistics*, New York: Academic Press, 600 p.

Kaplan, P.G., 1991, A formalism to generate probability distributions for performance assessment modeling, in: *High-Level Radioactive Waste Management, Proceedings of the 2nd International Conference*, Las Vegas, Nevada, dates, American Nuclear Society, LaGrange Park, Illinois, p. 1487-1490.

Kaplan, P.G., and L. Yarrington, 1989, Modeling the uncertainty in the parameter values of a layered, variably saturated column of volcanic tuff using the beta probability distribution, in: *Solving Ground Water Problems With Models*, papers from the NWWA conference, February 7-9, 1989, Indianapolis, IN, Association of Ground Water Scientists and Engineers, Indianapolis, IN, p. 111-128.

Kirkpatrick, S., C. Gelatt, Jr., and M. Vecchi, 1983, Optimization by simulated annealing: Science, v. 220, p. 671-680.

Larson, H.J., 1982, Introduction to probability theory and statistical inference, New York: John Wiley and Sons, 637 p.

Longenbaugh, R.S., C.A. Rautman, and E.E. Ryder, 1995, Yucca Mountain thermal response: An evaluation of the effects of modeled geologic structure and thermal property descriptions, *Sandia Report SAND94-2247*, Sandia National Laboratories, Albuquerque, New Mexico, 120 p.

Montezar, P. and W.W. Wilson, 1984, Conceptual hydrologic model of flow in the unsaturated zone, Yucca Mountain, Nevada: *U.S. Geol. Surv. Water-Resources Investigations Report 84-4345*, 55 p.

Ortiz, T.S., R. L. Williams, F.B. Nimick, B.C. Whittet, and D.L. South, 1985, A three-dimensional model of reference thermal-mechanical and hydrological stratigraphy at Yucca Mountain, southern Nevada: *Sandia Report SAND84-1076*, Sandia National Laboratories, Albuquerque, New Mexico, 71 p.

Rautman, C.A., 1990, Application of geostatistics to rock properties modeling at the Yucca Mountain nuclear waste repository site, Nevada: *Geol. Soc. Am. Abstracts with Programs*, v. 22, no. 6, p. 42.43.

Rautman, C.A., and A. H. Treadway, 1991, Geologic uncertainty in a regulatory environment: an example from the Potential Yucca Mountain nuclear waste repository site: *Environmental Geology and Water Science*, v. 18, p. 171-184.

Rautman, C.A., 1993, Direct probability mapping of contaminants, in: *Proceedings of ER'93 Environmental Restoration Conference*, Augusta, GA, October 24-28, 1993, p. 123-128.

Rautman, C.A., and A.L. Flint, 1992, Deterministic geologic processes and stochastic modeling, in: *High-Level Radioactive Waste Management, Proceedings of the 3rd International Conference*, Las Vegas, Nevada, April 13-17, 1992, American Nuclear Society, LaGrange Park, Illinois, p. 1617-1624.

Rautman, C.A., J.D. Istok, A.L. Flint, L.E. Flint, and M.P. Chornack, 1993, Influence of deterministic geologic trends on spatial variability of hydrologic properties in volcanic tuff, in:

High-Level Radioactive Waste Management, Proceedings of the 4th International Conference, Las Vegas, NV, April 26-30, 1993, American Nuclear Society, LaGrange Park, IL, p. 921-929.

Rautman, C.A. and T.H. Robey, 1993, Recent developments in stochastic modeling and upscaling of hydrologic properties in tuff, in: *High-Level Radioactive Waste Management, Proceedings of the 4th International Conference*, Las Vegas, NV, April 26-30, 1993, American Nuclear Society, LaGrange Park, IL, p. 1437-1445.

Rautman, C.A. and T.H. Robey, 1994, Development of stochastic indicator models of lithology, Yucca Mountain, Nevada, in: *High-Level Radioactive Waste Management, Proceedings of the 5th International Conference*, Las Vegas, Nevada, May 22-26, 1994, American Nuclear Society, LaGrange Park, Illinois, p. 2510-2519.

Rubin, Y., and J.J. Gomez-Hernandez, 1990, A stochastic approach to the problem of upscaling conductivity in disordered media: Theory and unconditional numerical simulations: *Water Resources Research*, v. 26, p. 691.

Sawyer, D.A., Fleck, R.J., Lanphere, M.A., Warren, R.G., and Broxton, D.A., 1990, Episodic volcanism in the southwest Nevada volcanic field: New $^{40}Ar/^{39}Ar$ geochronologic results [abs.]: EOS, Transactions, Am. Geoph. Union, v. 71, no. 42, p. 1296.

Sawyer, D.A., Fleck, R.J., Lanphere, M.A., Warren, R.G., Broxton, D.A., and Hudson, M.R., in press, Episodic caldera volcanism in the Miocene southwestern Nevada volcanic field, Revised stratigraphic framework, $^{40}Ar/^{39}Ar$ geochronology, and implications for magmatism and extension: *Geological Society of America Bulletin*, v. 106, p. 1304-1318.

Scott, R.B., and J. Bonk, 1984, Preliminary Geologic Map of Yucca Mountain, Nye County, Nevada, with Geologic Sections: *U.S. Geol. Survey Open-File Report 84-494*.

Scott, R.B., and M. Castellanos, 1984, Stratigraphic and structural relations of volcanic rocks in drill holes USW GU-3 and USW G-3, Yucca Mountain, Nye County, Nevada: *U.S. Geol. Surv. Open-File Report 84-491*, 121 p.

Soeder, D.J., L.E. Flint, and A.L. Flint, 1991, Effects of sample handling and measurement methodology on the determination of porosity in volcanic rock samples: Agronomy Abstracts, 1991 Annual Meetings, Am. Soc. Agronomy, Crop Sci. Soc. Am., Soil Sci. Soc. Am., p. 232.

Spengler, R.W., F.M. Byers, Jr., and J.B. Warren, 1981, Stratigraphy and structure of volcanic rocks in drill hole USW-G1, Yucca Mountain, Nye County, Nevada, *U.S. Geol. Survey Open-File Report 81-1349*, 50 p.

Suro-Perez, V., and A.G. Journel, 1991, Indicator principal component kriging: *Mathematical Geology*, v. 23, p. 759-788.

Tidwell, V.C., 1994, Scaling behavior of gas-permeability measurements in volcanic tuff, in: *High-Level Radioactive Waste Management, Proceedings of the 5th International Confer-*

ence, Las Vegas, Nevada, May 22-26, 1994, American Nuclear Society, LaGrange Park, Illinois, p. 2500-2509.

USGS (U.S. Geological Survey, Rock Characteristics Section), 1993, Methodology and source data used to construct the demonstration lithostratigraphic model. Second progress report: *Milestone Report 3GGU134M*, U.S. Department of Energy, Yucca Mountain Project, Las Vegas, NV, 30 p.

Wilson, M.L., J.H. Gauthier, R.W. Barnard, G.E. Barr, H.A. Dockery, E. Dunn, R.R. Eaton, D.C. Guerin, N. Lu, M.J. Martinez, R. Nilson, C.A. Rautman, T.H. Robey, B. Ross, E.E. Ryder, A.R. Schenker, S.A. Shannon, L.H. Skinner, W.G. Halsey, J. Gansemer, L.C. Lewis, A.D. Lamont, I.R. Triay, A. Meijer, and D.E. Morris, 1994, "Total-System Performance Assessment for Yucca Mountain -- SNL Second Iteration (TSPA-93)," *Sandia Report SAND93-2675*, Sandia National Laboratories, Albuquerque, New Mexico.

Winograd, I.J., and W. Thordarson, 1975, Hydrogeologic and hydrochemical framework, south-central Great Basin, Nevada-California, with special reference to the Nevada Test Site: *U.S. Geol. Surv. Prof. Paper 712-C*, 126 p.

Xu, W., T. Tran, R.M. Srivastava, and A.G. Journel, 1992, Integrating seismic data in reservoir modeling: The collocated cokriging alternative: *SPE Paper 24742*.

Zhu, H, 1991, Modeling mixtures of spatial distributions with integration of soft data: Ph. D. thesis, Stanford University, Stanford, CA.

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