An essential part of the license application for a geologic repository will be the demonstration of compliance with the standards set by the Environmental Protection Agency. The performance assessments that produce the demonstration must rely on models of various levels of detail.

The most detailed of these models are needed for understanding thoroughly the complex physical and chemical processes affecting the behavior of the system. For studying the behavior of major components of the system, less detailed models are often useful.

For predicting the behavior of the total system, models of a third kind may be needed. These models must cover all the important processes that contribute to the behavior of the system, because they must estimate the behavior under all significant conditions for 10,000 years. In addition, however, computer codes that embody these models must calculate very rapidly because of the EPA standard's requirement for probabilistic estimates, which will be produced by sampling thousands of times from probability distributions of parameters. For this reason, the total-system models must be less complex than the detailed-process and subsystem models.

The total-system performance is evaluated through modeling of the following components:

- Radionuclide release from the engineered-barrier system.
- Fluid flow in the geologic units.
- Radionuclide transport to the accessible environment.
- Radionuclide release to the accessible environment and dose to man.

The relationship among these components is shown in Figure 1. Each of these components is modeled at more than one level of detail. The levels of detail of performance-assessment models form a model hierarchy, which can be envisioned as a triangle with the most complex models forming the base and the least complex models near the apex (Figure 2). The most complex models are process models; the least complex are systems models, and the intermediate are subsystem models, sometimes called domain models. For visualization purposes the hierarchy of models can
Figure 1. Components of Total-System Performance Assessment
Figure 2. Hierarchy of Models Used in Performance Assessment
be thought of as being composed of three levels. The levels are not completely distinct; a single model may sometimes be thought of as in one level and sometimes in another, depending on how it is used. The division between process and subsystem models, however, is especially indistinct. For this reason the boundary between process and subsystem models has been shown as a dashed line on Figure 2.

Process models are usually deterministic numerical codes that incorporate coupled interactions such as the interactions among water, water vapor, gas, and heat flow. These models closely represent the physical (chemical) processes that occur and are used to evaluate the effects of parameter uncertainty by conducting parameter sensitivity analyses over the ranges of model input parameters that exist at the site.

Subsystem models are either deterministic or probabilistic models, which are used in analysis of individual sequences of processes and events that may occur at a repository site, bounding analyses, or determinations of process uncertainty. An example of a subsystem model is the waste-package model, which incorporates chemical/geochemical, flow, stress, and thermal processes in an abstracted (simplified) form. Subsystem models are used to investigate process uncertainty through incorporation of the range of expected processes that could occur at the site.

System models are capable of describing combinations of potential site scenarios (i.e., sequences of processes and events that could occur at a site); they can be used to estimate the effects of these combinations on the entire repository system. Because they generally treat the combinations probabilistically, they are useful in calculating complementary cumulative distribution functions for examining compliance with 40 CFR Part 191. These models, in comparison with the rest of the hierarchy, incorporate the highest levels of abstraction.

The base of the hierarchy of models used in performance assessment (Figure 2) is thought of as containing models that are more complete. Toward the apex, models contain all of the major components of models at the base, but process descriptions are in an abstracted (less detailed) form. For this reason, the models toward the apex are useful in showing the sensitivity of the system to variations in the parameters that describe processes and events. The models toward the base are useful in deriving information about the effects of uncertainties in those parameters.

Iterative assessments of total-system performance can be envisioned as beginning at either the base of the triangle or the apex. Useful transfers of information between levels of the hierarchy may be accomplished either upwards or downwards in the triangle. When information is passed upwards, the results of studies with process models may formulate input for subsystem models, whose results are in turn used as a basis for calculations with system models. In this way the uncertainties
in the detailed modeling of phenomena are passed up to the system models, which can then take those uncertainties into account in examining compliance with regulations. When information is passed downwards, sensitivity studies with system models can identify the phenomena that contribute most significantly to system performance and therefore require detailed investigation with process models.

A single complete iteration of performance-assessment calculations is likely to pass information in both directions. Because the comparisons with regulations are generally made with the system models near the apex, it is important for each iteration to ensure that the results of the system models are consistent with the less abstracted models toward the base. (Iterations after the first do not need to repeat all the calculations: the process-model results generally need to be recalculated only if new data or a change in the set of scenarios extend the range of a parameter beyond the analyses conducted for the first iteration.) Exercising the hierarchy of models in these ways aids in understanding the interrelationships among the levels of complexity of the models; this understanding is essential to obtaining reasonable assurance in the demonstrations of compliance with regulations.

The series of iterative performance assessments for the Yucca Mountain site began in 1991 with a total-system performance assessment in which largely system and subsystem models were exercised.\(^2\) The complexity of the modeling approach will increase with each iteration, and results will be used to guide site characterization and design, to guide model development, and to provide a basis for interactions with the NRC and the public.

For each iteration, information from other components of the repository programs is used; the performance assessment is conducted; and the results are disseminated among the components of the program. Figure 3 shows the interactions between performance assessment and the other components of the repository program (e.g., regulation, design, site characterization, model development, and the public). This process can be thought of as information being fed in, analyses being conducted, and information being fed out to the components with each iteration (Figure 3). In this way, the results of performance assessment are used to influence design and site characterization and to present results to the NRC and the public with each iteration. The NRC and public comments will be considered in developing the scope of the next iteration. Results at each level in Figure 2 may be calculated with each iteration, where necessary, as new data, scenarios, and models become available during the iterative process.

A number of total-system models have been developed and used for studies of the behavior of a potential repository at Yucca Mountain, Nevada. An example of the highest level, most abstracted of the system models is embodied in a computer
Figure 3. Interactions Between Performance Assessment and Other Components of the MGDS Program for Each Iteration
spreadsheet, developed by L. Rickertsen and as yet not documented. This code uses simple numerical descriptions of processes and does not do any calculation beyond arithmetic. It is most effective when used in trade-off analyses or in decision analyses at the least detailed level. A code of this type offers complete portability, is completely transparent to the user and the public, and is easy to use.

The next level of complexity can be described by the code RIP, developed by Golder Associates. This code is a shell for probabilistic calculations. As most often used, the shell can change its abstractions of lower-level models by changing sets of data that usually are distribution functions. This code can be used effectively in trade-off and compliance studies at a more detailed level than the spreadsheet model. It is of limited usefulness in evaluating the effects on particular processes when the parameters that describe them change.

Still more elaborate in several respects is a total-system, model developed by the Electric Power Research Institute. In addition to distribution functions, the code contains simple process models. In practice, the code generally works with only a few discrete values chosen from probability distributions rather than with convolutions of the distributions. For this reason, calculations of a process are usually described by a finite number of outcomes, each with a discrete probability.

Also used as total-system models are the computer codes TOSPAC developed at Sandia National Laboratories and SUMO developed at Pacific Northwest laboratory. These codes include more complex abstractions of the hydrologic models and a model of releases of radionuclides from waste packages. Because these codes perform relatively complex calculations, they may not be as useful for probabilistic estimates that must rely on many thousands of computer runs. They were the major tools used in the probabilistic assessments of total-system performance carried out in 1991.

A good example of a subsystem models is the waste-package model AREST. This model is made up of three submodels; a waste-package containment model, a waste-package release model, and an engineered-system release model. The containment model simulates the degradation of the metallic barriers of the package by uniform corrosion, pitting, and stress corrosion in the presence of heat, radiation, and mechanical stress. The waste-package release model, upon package failure, simulates the release of radionuclides and their migration out through the package. The engineered-system-release model integrates individual waste-package releases to obtain estimates of total release from the engineered-barrier system to the host rock. The AREST model is also an example of the lack of firm distinction between levels in the hierarchy; it is sometimes used as a "less complex" model because it is simple enough to use analytical solutions to the equations that describe the phenomena it models.
Process models are more complex and are normally based on a formulation of governing equations based on the laws of physics. Only two examples of process models will be presented here: the code TOUGH developed by LBL and the code TRACR3D developed at LANL. TOUGH\(^6\) is a multidimensional numerical code that simulates the coupled flow of water, vapor, air, and heat through porous and fractured media. TRACR3D\(^9\) is a multidimensional flow and transport code that simulates the flow and transport of radionuclides through the unsaturated zone in water, vapor, and air in the absence of thermal loading.

The first iteration of total-system performance assessment was an example of the exercise of the model hierarchy. The system models were chosen from near the apex of the hierarchy, while calculations in support of the use of those models were performed with models near the base of the hierarchy. None of the higher level models explicitly considered the effects of thermal loading on the unsaturated ground-water flow. (Thermal effects on gas flow were considered.) In other words, the system models were abstracted from isothermal flow models. The next iteration may continue the exercise of the hierarchy by developing abstractions from nonisothermal models such as those embodied in TOUGH or TRACR3D.


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