

Assessment of Effectiveness of
Geologic Isolation Systems

**A Short Description of
the AEGIS Approach**

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September 1980

Prepared for the
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by Battelle Memorial Institute



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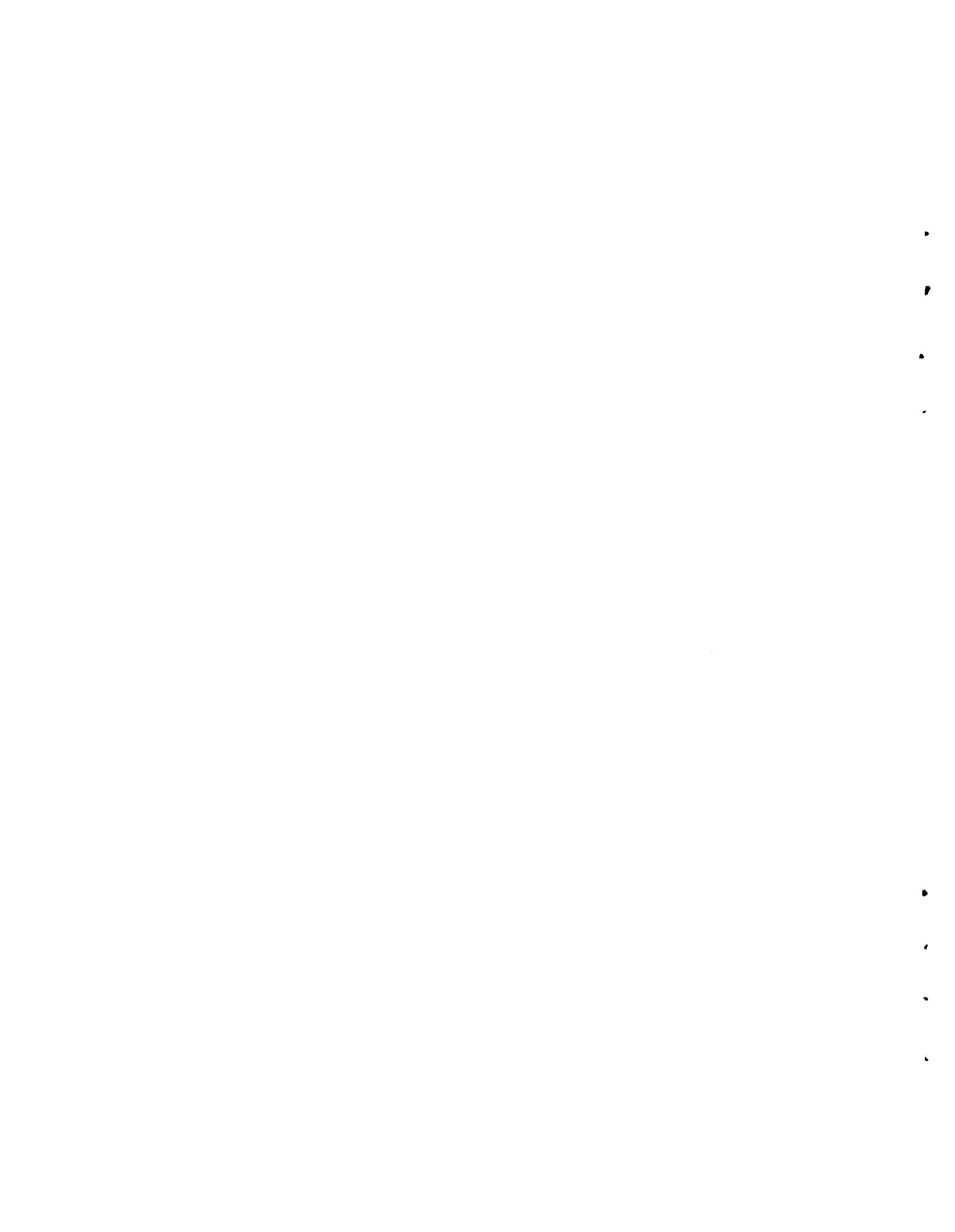
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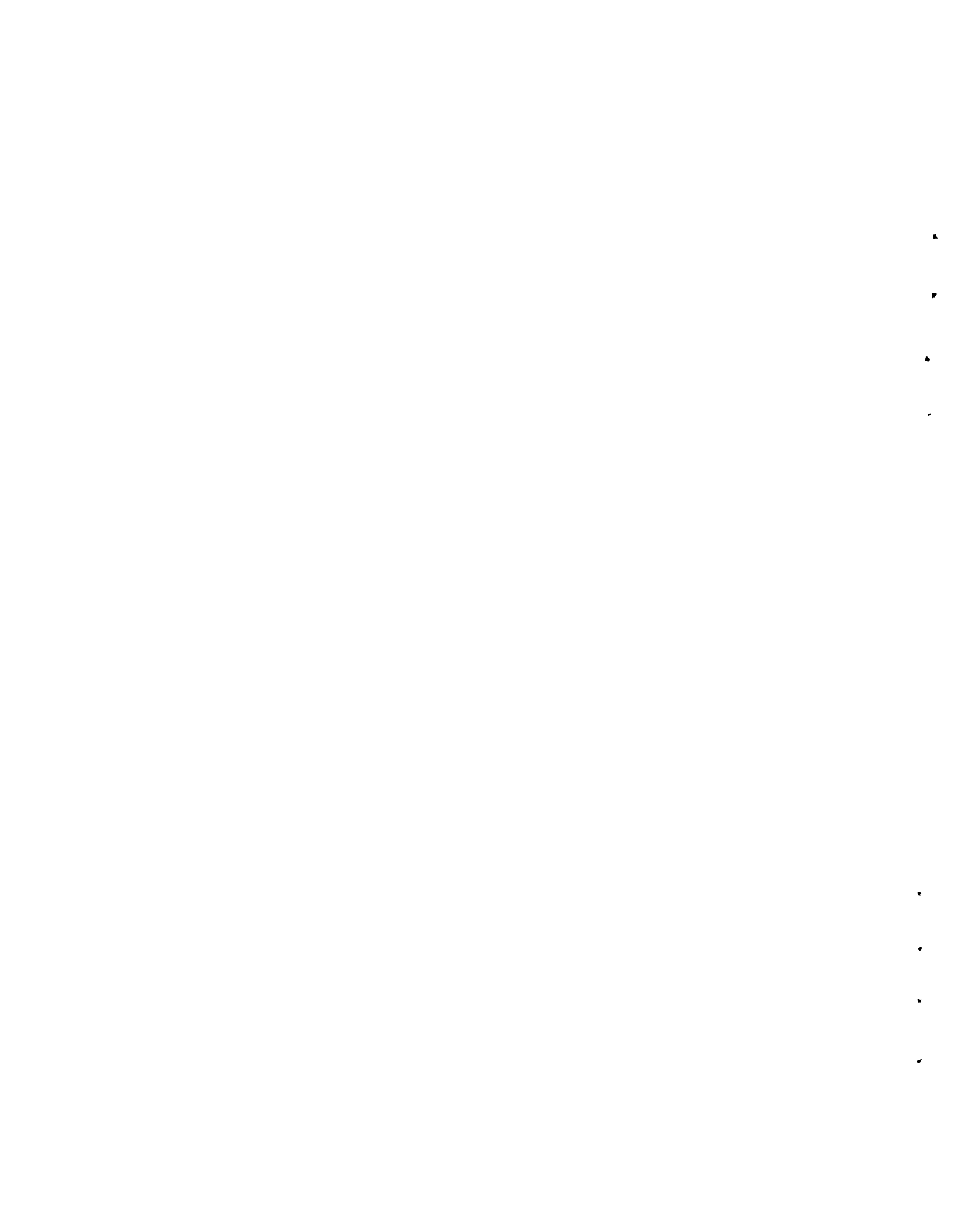
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INTRODUCTION

The commercial production of nuclear power produces potentially hazardous high-level nuclear waste. This waste may be in the form of spent fuel, or result from the reprocessing of spent fuel. The placement of radioactive wastes in deep geological repositories is being considered as a disposal method which would effectively isolate these wastes from the environment for long periods of time. In the United States, the Department of Energy (DOE) is seeking to develop these deep geological repositories. However, before they can be used for the disposal of nuclear waste, federal legislation requires that they must be licensed by the Nuclear Regulatory Commission (NRC) and meet radiation protection standards being established by the Environmental Protection Agency (EPA).

To meet these licensing criteria and protection standards, research programs are in progress to determine acceptable waste forms, canisters to contain the waste, backfill materials to fill the void spaces in the mined repository, and the geological formations which isolate the repository from the accessible environment. These components, in combination, comprise a system for disposal of high-level waste. While specific performance criteria may be imposed on individual components, the ultimate test of the repository will involve an evaluation of the total geologic isolation system as a unit. Therefore, methods must be developed to evaluate the effectiveness of the total system. To meet this need, the Pacific Northwest Laboratory has been developing and improving methods to assess the long-term effectiveness of isolating nuclear wastes in geologic formations. This work was started in 1976 in the Waste Isolation Safety Assessment Program (WISAP) and continues in the Assessment of Effectiveness of Geologic Isolation Systems (AEGIS) Program.

The evaluation of this long-term effectiveness involves a number of distinct steps. Initially, the specific nature of the engineered components in the repository and of the existing geologic and hydrologic systems surrounding the repository must be adequately understood. Since natural geologic processes and future human activities may alter these systems over the long time frames necessary for isolation, an evaluation must also be made to determine if there

are plausible scenarios for breaching the repository. If such a scenario is identified, then the transport of radionuclides from the repository to the environment must be estimated. A final step can be added to estimate the effects of the radionuclides in the environment.

AEGIS currently has the methods for performing these evaluation steps. These methods are continuously being improved to meet the increasing level of sophistication which will be necessary as more data are acquired and as the site selection and licensing process develops. The existing AEGIS approach is to obtain the necessary information which characterizes the geologic isolation system from the programs designing the engineered components and the programs making field measurements of the geology and hydrology. AEGIS then develops a conceptual description of the geologic systems and uses computer models to simulate the existing ground-water pathways. AEGIS also uses a team of consulting experts, with the assistance of a computer model of the geologic processes, to develop and evaluate plausible release scenarios. Then other AEGIS computer models are used to simulate the transport of radionuclides to the surface and the resultant radiation doses to individuals and populations. The purpose of this report is to describe this approach. Technical details of specific aspects of the AEGIS approach may be found in the reports identified in Appendix E.

ASSESSMENT APPROACH

An important feature of the AEGIS approach is that it can operate at various levels of sophistication depending on the amount of information available. During the site selection and evaluation phase only preliminary assessments will be necessary. However, in later phases of site selection and licensing, more detailed information will be provided and AEGIS will be required to perform more thorough assessments with greater accuracy and reduced uncertainty. Therefore, the methods used in the AEGIS program are being developed to be flexible, thorough, objective, and scientifically defensible.

The AEGIS approach for evaluating the effectiveness of a geologic repository is identified in Figure 1. Each step in this figure is expanded in the following discussion. These steps have been applied at various levels of sophistication for a hypothetical repository in bedded salt (PNL-2782, PNL-3070), in a salt dome (PNL-2955), and in basalt (in preparation).

STEP 1: ACQUIRE INFORMATION ON THE GEOLOGIC, HYDROLOGIC AND ENGINEERED SYSTEMS OF THE PROPOSED REPOSITORY SITE

The first step involves a search and compilation of all the available geologic, hydrologic, and geochemical information for the region being studied. Much of this information is obtained from sources such as federal and state publications, DOE sponsored programs, or from geologic project managers who are actively involved with identifying and characterizing the geologic and hydrologic properties of a particular geologic medium. Additional information is acquired from other agencies and the scientific literature. Information is also obtained from consultants who, along with our staff, analyze the data, identify future data requirements, and suggest and implement further research efforts. Because ground water is the most probable transport medium for radionuclides from deep underground repositories, the local and regional geology and hydrology must be evaluated. This involves identifying the various aquifer systems, their hydrologic characteristics, and the recharge and discharge locations.

Of equal importance is understanding the geologic history of the region by determining the various rock types, their distribution in the area, and the

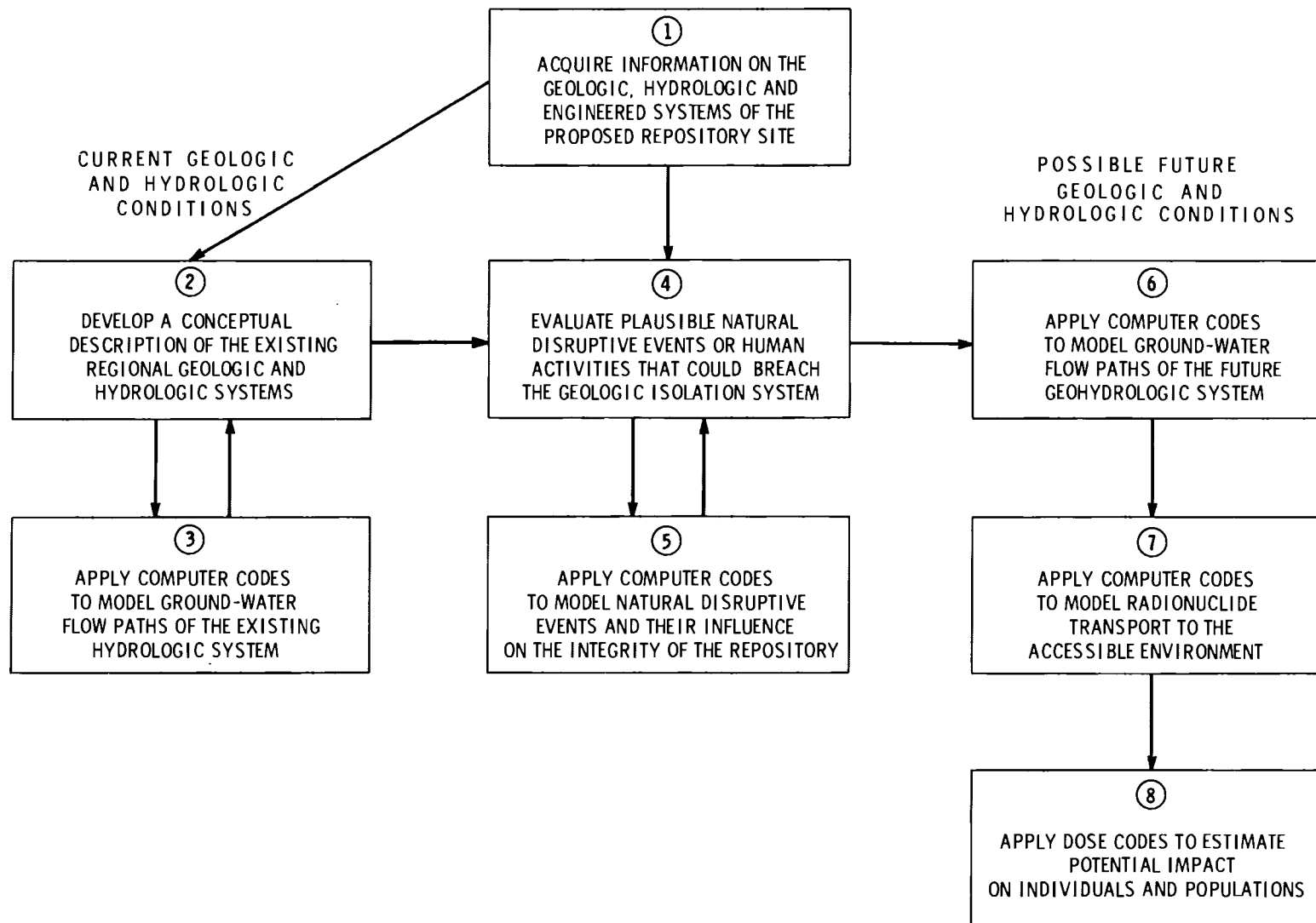


FIGURE 1. Assessment Flow Diagram

regional and local structural features. Insights into future evolution of the region can be obtained from the specific regional information. This understanding of the geology and consideration of natural geologic processes operating on the region provide the basis for a conceptual geohydrologic description of the repository site and region.

Additional information involving the influence of geochemical effects on the integrity of the repository is currently being investigated. This information includes a chemical analysis of the ground water and the mineral types that may contact the ground water. This information also provides insight into the origin and source of ground water, residence time, and chemical evolution of the ground-water system.

Information is also acquired from programs designing the engineered systems of the repository. This includes the quantity and type of radionuclides in the inventory, and characteristics of the waste form, waste canister, additional engineered barriers, and the repository dimensions and design.

STEP 2: DEVELOP A CONCEPTUAL DESCRIPTION OF THE EXISTING REGIONAL GEOLOGIC AND HYDROLOGIC SYSTEMS

The second step for applying the AEGIS approach to a specific site involves the preparation of a conceptual description of the geologic and hydrologic systems in cooperation with geologic project managers. An example of a simplified geologic cross section for the bedded salt study is presented in Figure 2.

The result is a composite description of the region, which should include potentiometric maps, structure maps for the various geologic and hydrologic units, pumping and recharge distributions, and boundary conditions. Often this information must be interpolated based on available data from drilling logs, static well measurements from the same aquifer, topographic maps, meteorological measurements, stream flow records, etc. Specific information, which must sometimes be interpreted from incomplete data, includes: 1) the locations and amounts of ground-water recharge and discharge at geologic formation outcrops and perimeters, and 2) the hydraulic connections between deep confined aquifers, shallow unconfined aquifers, and surface water systems.

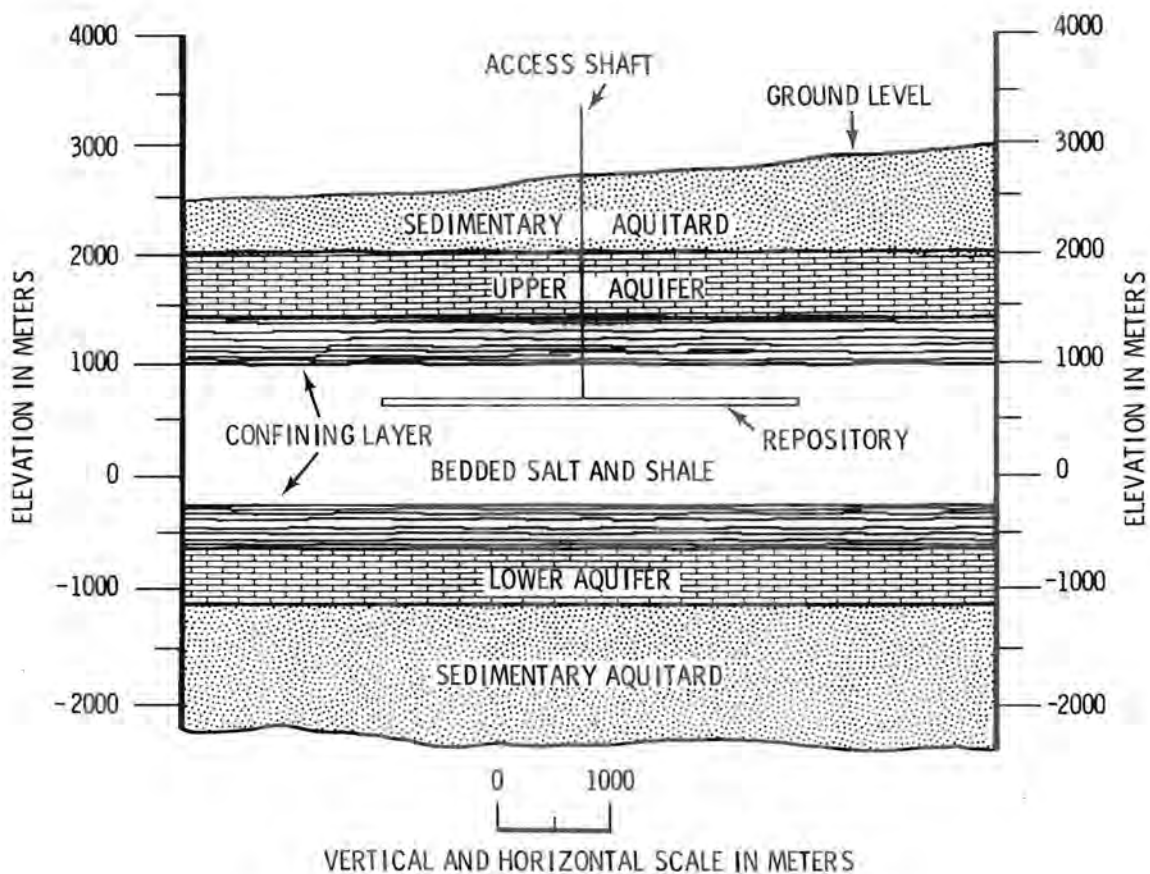


FIGURE 2. Simplified Geologic Cross Section

In addition to the geologic and hydrologic descriptions, the geochemical aspects of the geosystem must also be characterized. However, most of this information will be provided by other DOE sponsored programs actively involved with determining the characteristics of the source terms (waste radionuclides) and their solubility and behavior in ground water.

STEP 3: APPLY COMPUTER CODES TO MODEL GROUND-WATER FLOW PATTERNS OF THE EXISTING HYDROLOGIC SYSTEM

After the conceptual description of the specific repository site and region has been developed, computer codes are used to model flow patterns within the hydrologic system. The Variable Thickness Transient ground-water hydrologic code (VTT) is one of the AEGIS codes used for modeling ground-water flow patterns. It is a two-dimensional code that can simulate multiaquifer systems in

a heterogeneous geology. For more detailed multilayered systems, the fully three-dimensional Finite-Element 3-D Ground-Water code (FE3DGW) is used to define more precisely ground-water flow patterns. The VTT and FE3DGW codes provide a flexible and efficient method to handle complex aquifer systems using either limited or extensive data.

An important characteristic of the AEGIS computer code usage is the interactive computer system at PNL. Interactive computer systems allow the user to receive essentially immediate response from the computer, greatly enhancing the feedback between the user and the computer. Since the AEGIS computer codes must be adapted to model the conceptual description of the particular repository region, the interactive computer system used by AEGIS makes that process much more efficient and, more importantly, substantially increases the involvement of geoscientists and hydrologists in the AEGIS computer operations. Thus, the output from these codes can be readily used to evaluate and refine the conceptual description of the geologic and hydrologic systems in the region to make the results compatible with observed data. A more detailed description of the various hydrologic codes can be found in Appendix A.

STEP 4: EVALUATE PLAUSIBLE NATURAL DISRUPTIVE EVENTS OR HUMAN ACTIVITIES THAT COULD BREACH THE GEOLOGIC ISOLATION SYSTEM

The geology of the region surrounding a repository will continue to change because of the natural processes operating over the long time frames needed for isolation. Projections of the possible evolutionary paths can be made based on the geologic history of the region, the existing states of the geologic and hydrologic systems, and the scientific understanding of the geologic processes in effect. AEGIS uses the conceptual description of the existing geohydrologic system as a focus for evaluating future states of the system. The expertise of a team of consultants is used by the AEGIS staff to help characterize the natural processes which could affect the repository located in a particular geologic formation. A computer model is used to assist the AEGIS staff in keeping track of the large numbers of natural processes, as described in Step 5. Other information is used to identify potential human activities and waste-induced phenomena which could affect the integrity of a repository.

Based on these considerations, AEGIS identifies and quantifies plausible breach scenarios that need to be further analyzed. AEGIS seeks to provide an auditable method for the derivation and quantification of such scenarios, with estimates of the plausibility and time of occurrence. In this process of developing scenarios, AEGIS can also provide the justification for discarding other scenarios as being implausible.

STEP 5: APPLY COMPUTER CODES TO MODEL NATURAL DISRUPTIVE EVENTS AND THEIR INFLUENCE ON THE INTEGRITY OF THE REPOSITORY

One aspect of the scenario evaluation step for which computer simulation is particularly useful is the combining of all the many natural potential disruptive events into sequences of events that might lead to a repository breach. The AEGIS release scenario computer code consists of many submodels, each simulating individual natural processes over time. These submodels treat such natural processes as faulting, climatic changes, volcanism, flooding, subsidence, erosion, and others. The logic within each submodel represents the current understanding of these processes. Since many of the processes cannot be predicted precisely, the submodels include functions of the probability of an event versus its magnitude. The functions are derived from data and subjective probabilities from expert consultants.

At each point in time during a simulation run, values for the processes are selected at random from these functions, providing a probabilistic treatment of the natural events. A single simulation run over time identifies just one of the very many possible futures for the geologic system. The AEGIS release scenario code is used to make many simulation runs to illustrate various possible states of the geologic system with some indication of their relative likelihood of occurrence. Thus this approach, called a Monte Carlo technique, is a bookkeeping tool for systematically inspecting possible geological futures.

This unique AEGIS code has been especially designed to maximize its flexibility so that the logic and data can be directly altered by experts to match the state of the art knowledge about geologic processes and to match the particular characteristics of each region. This process is aided substantially by the interactive nature of the computer system. The output from this code is

evaluated by the AEGIS staff and consultants in the development and selection of particular breach scenarios (Step 4). For more information on this code, refer to Appendix B.

STEP 6: APPLY COMPUTER CODES TO MODEL GROUND-WATER FLOW PATHS OF THE FUTURE HYDROLOGIC SYSTEM

If the repository release scenario model identifies an event or series of events that cause a breach of the repository, then the input data for the ground-water flow codes are updated as required by the description of the release scenario. The information obtained from the ground-water models is then used for input into radionuclide transport codes (Step 7).

STEP 7: APPLY COMPUTER CODES TO MODEL RADIONUCLIDE TRANSPORT TO THE ACCESSIBLE ENVIRONMENT

The codes used for radionuclide transport, like the ground-water codes, are multi-dimensional and interactive. A one-dimensional version of the Multicomponent Mass Transport Model (MMT) is the code currently used for the AEGIS applications.

MMT1D simulates migration of radionuclides along a one-dimensional flow path, at the same time accounting for the radioactive decay of the nuclides. Radionuclide-geologic media interaction is simulated by a distribution coefficient (Kd). The Kd is a measure of the ability of a geologic media to retard a given radionuclide. In addition to distribution coefficients, other input includes:

- ground-water flow velocity
- longitudinal dispersivity
- flow path length
- dimensions of the stream tube
- nuclide half-lives
- a matrix describing radionuclide chain decay
- porosity
- leach rate information.

Information obtained from examining the geochemical properties of the ground-water and rock types is also useful for providing insight into the interpretation of these input data.

A more complete description of the MMT code can be found in Appendix C.

STEP 8: APPLY RADIATION DOSE CODES TO ESTIMATE POTENTIAL IMPACT ON INDIVIDUALS AND POPULATIONS

When radionuclides are released to the atmosphere or to surface waters, they may disperse or may accumulate in the environment. Even short-term (acute) releases can lead to long-term environmental contamination, which in turn leads to long-term irradiation of individuals and populations. Pathways of human exposure to these radionuclides include direct radiation from contaminated air, water, sediment, and soil; ingestion of contaminated drinking water, aquatic food products, terrestrial farm crops, and farm animal products; and inhalation of airborne materials. These exposure pathways are evaluated using the computer programs KRONIC, SUBDOSA, DACRIN, ARRRG, FOOD, and PABLM. Site-specific information about demography, local crop production practices, eating habits, and recreational activities is required input for these codes.

The computer programs KRONIC and SUBDOSA can be used to compute doses from direct irradiation from a passing plume of radionuclides. KRONIC is used with average annual meteorology information to determine doses from chronic events. SUBDOSA is used to calculate doses from short-term exposure to a plume of radionuclides. The program DACRIN can be used to calculate the dose from inhalation of airborne material from both acute and chronic releases.

The program ARRRG can be used to compute internal doses from ingestion of drinking water, fish, other aquatic animals, or aquatic plants, as well as external doses from swimming, boating, and shoreline exposure. Water concentrations of radionuclides are calculated in ARRRG as a function of nuclide release rate, effluent flow rate, and the mixing and dilution in the receiving waters. The doses calculated are a one-year dose and the 50-year dose from one year of ingestion.

Internal doses from ingestion of contaminated farm crops and animal products can be calculated with the program FOOD. The food products may be contaminated either by atmospheric deposition or irrigation with contaminated water. Air concentrations are input from codes such as KRONIC or SUBDOSA, and water concentrations are calculated as in ARRRG. Like ARRRG, doses calculated are a one-year dose and a 50-year dose from one year of exposure.

For those cases where it is more appropriate to calculate a total integrated lifetime dose from continuous exposure to changing levels of environmental contamination, the program PABLM can be used. PABLM combines the pathway modeling capabilities of both ARRRG and FOOD and can be used to calculate a dose from one year of exposure as well as a total integrated dose.

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APPENDIX A

HYDROLOGIC CODES FOR GROUND-WATER FLOW PATHS,
POTENTIALS, AND TRAVEL TIMES

NAME OF CODE: FINITE-ELEMENT THREE-DIMENSIONAL GROUND-WATER (FE3DGW)

DESCRIPTION

This three-dimensional, finite-element ground-water model determines ground-water potentials, flow paths, and travel time in a given complex multi-layered system. The simulated results are a function of stratifications, geologic properties, and hydrologic boundary conditions of the modeled region.

The repository sites might, for example, consist of a multi-aquifer system separated by confining layers in which the aquifers respond conjunctively to stresses imposed on each other. This three-dimensional model provides a realistic means of representing multi-layered aquifers associated with the geologic configuration. Since this is a finite-element model, it provides a powerful tool for defining the irregular boundaries of a complex geologic system and the associated surface water bodies. It also accounts for varying withdrawal, recharge, and infiltration rates, both in space and time domain.

FE3DGW has been designed for simulation of the large natural systems. It is capable of modeling the geologic systems by varying both the number and thickness of the layers. The point and distributed withdrawals and recharges are considered. The region modeled can also be conveniently subdivided for greater detail in critical localized areas.

In FE3DGW, the core storage requirements are reduced by both an efficient data organization on a disc for sequential retrieval and the use of a partially compressed matrix for solution of the associated sparse and unbanded system of equations. This reduces the core storage requirements for a three-dimensional solution to the extent that large natural systems can be simulated efficiently on small computers by FE3DGW. To minimize the cost of computation for a three-dimensional ground-water flow, the immediate results are stored for repeated retrieval at a fraction of the computational cost.

Input Data

Input data include both geologic and hydrologic details. To simplify the input data preparation for mathematical description of complex geologic systems,

three-dimensional finite elements are generated by FE3DGW using well-log descriptions. The following hydrogeologic parameters are also needed:

- well log data describing stratifications or interpolated contour map describing each hydrogeologic unit
- demarcation of surface water bodies, fault zones, and other natural or man-made features affecting ground-water flow
- hydraulic properties of each geologic layer
- flow conditions at the regional boundaries
- withdrawal and injection rates
- time-variant and steady-state water level in rivers, lakes, and regional boundaries
- land use, precipitation, and climatic data.

Model Output

To verify the data and results and to provide for interaction among appropriate scientific disciplines, FE3DGW and its supportive programs generate the following file and graphical outputs:

- plots of regional geometry and finite-element grid
- vertical geologic section at each node of the system
- plots of thickness, top and bottom elevations of each hydrogeologic system
- ground-water potential
- contour maps of:
 - potentials at the top and bottom of each hydrogeologic unit
 - potentials at a given elevation
 - differences in potentials between two hydrogeologic units
 - differences between two runs
 - vertical sections of interest.

The model also generates:

- files of ground-water potentials
- the flux rate at the center of each element of each layer
- streamline or pathlines defining flow path and travel times.

USES OF THE MODEL

The model can be used to simulate and solve a variety of problems (Gupta and Tanji 1976; Gupta and Pinder 1978). To illustrate some of the capabilities of the model, a typical problem is described below.

Hypothetical Repository for Radioactive Waste in Hard Rock

Figure A-1 shows the model's representation of a repository for radioactive waste in hard rock. The model was used to determine the flow paths and travel time of fluid moving from a repository in hard granitic rock or gneiss that has small fracture planes or joints that are interconnected. Lakes, rivers, and topography of the area are represented in Figure A-2. The element size, shape, and orientation are set to account for surface-water bodies, topography, and structural properties of the region. The major fracture zones are represented and discrete elements with two additional thin elements represent major fracture zones and provide a transition zone from fractures to the rock matrix (Figure A-1).

To predict streamlines and travel time, an auxiliary program, TVL3D, was used. Figure A-3 shows the X-Y plane plot of the streamlines from the middle (5), left (3), and right (4) corners of the hypothetical repository. Figure A-4 is the plot of X-Z paths of the streamlines.

VERIFYING THE CODE WITH ANALYTICAL SOLUTIONS

The following analytical solutions were used to verify transient and steady-state results:

- THEIS nonequilibrium equation defining unsteady radial flow to a well, pumping at a constant rate in an infinite, homogeneous, and isotropic aquifer (Theis 1935).

- PATHS code based on an analytical solution defining the potential distribution in an aquifer system having an initial uniform gradient, large remote radial boundary, and cavernous (cylindrical) reservoirs (Nelson and Schur 1980).
- HANTUSH solution defining drawdown distributions in the vicinity of a steady well draining an elastic artesian aquifer confined by semipervious elastic strata (Hantush 1959).

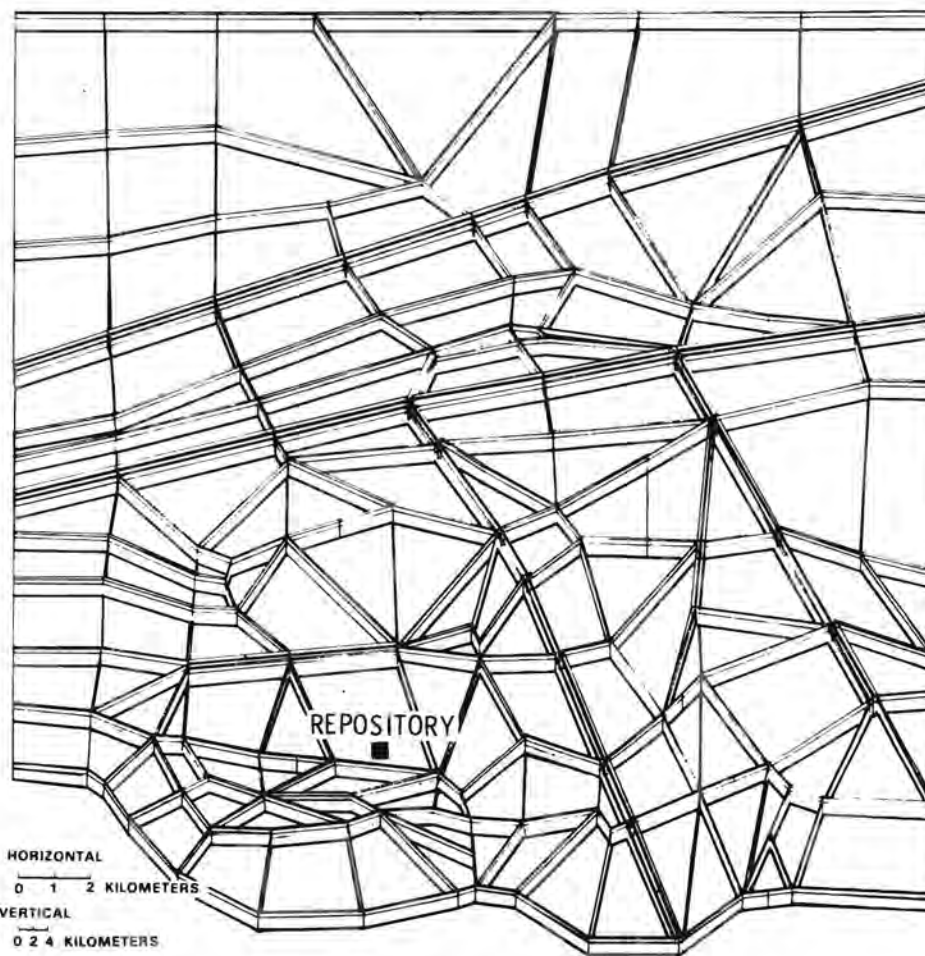


FIGURE A-1. FE3DGW Representation of a Repository in Granite

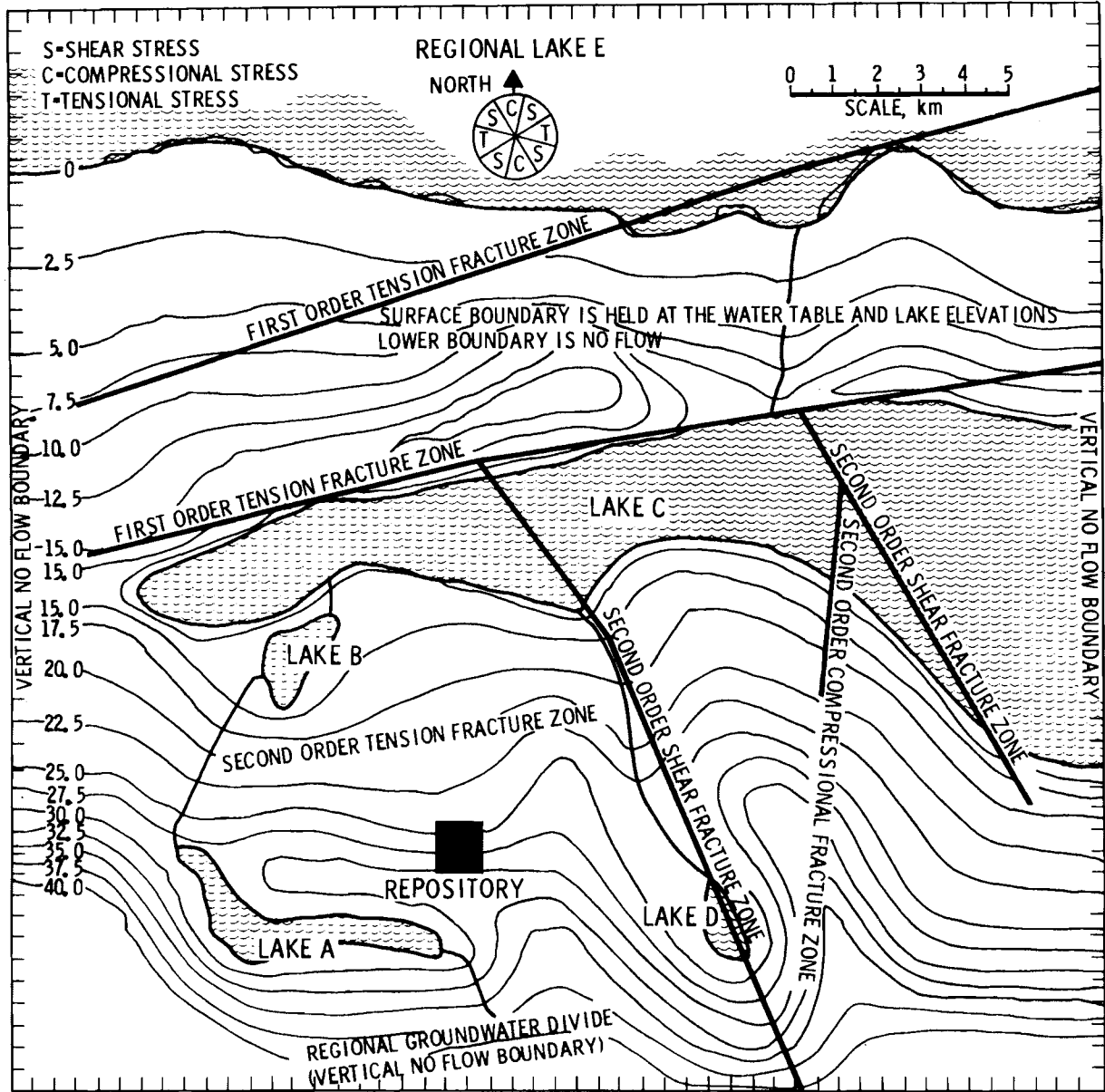


FIGURE A-2. Reference Repository Site in Granite, Illustrating Boundaries, Fractures and Water Table

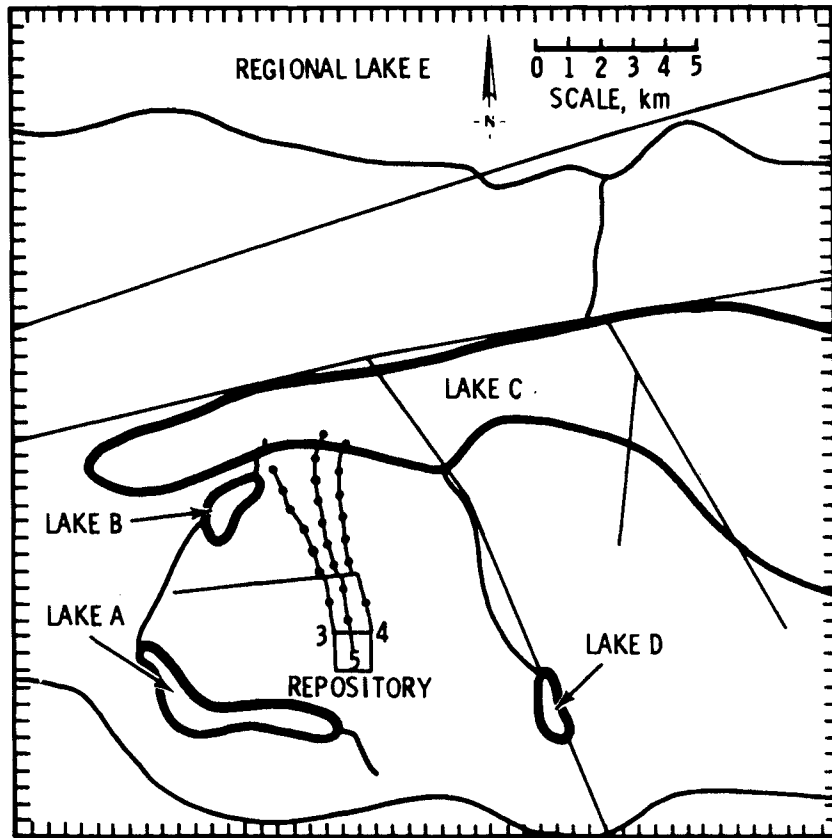


FIGURE A-3. X-Y Plane Plot of Streamlines for a Hypothetical Repository in Granite Starting From Middle (5), Upper Left (3), and Upper Right (4) Corners of Repository. (The dots on the streamlines are 1,000 years apart.)

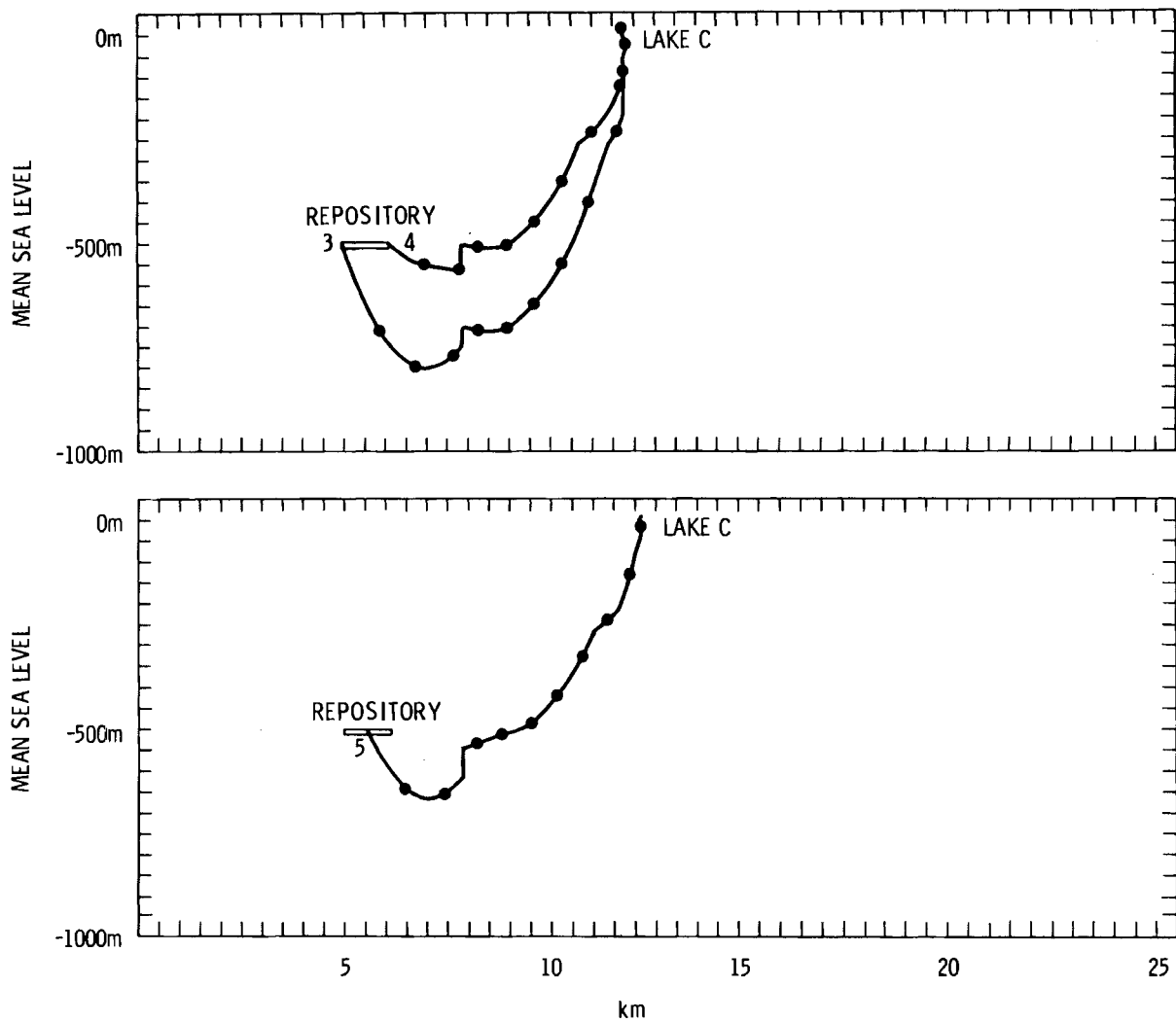


FIGURE A-4. X-Z Plane Plot of Streamlines from a Hypothetical Repository in Granite Starting From Middle (5), Upper Left (3), and Upper Right (4) Corners of Repository. (The dots on the streamlines are 1,000 years apart.)

NAME OF CODE: VARIABLE THICKNESS TRANSIENT GROUND WATER (VTT)

DESCRIPTION

The VTT code is used to study changes in the potentiometric surface by simulating the flow of an incompressible fluid that saturates a rigid, porous soil matrix. It can describe saturated ground-water flow in unconfined and confined aquifers and can handle multi-aquifer systems with interaquifer transfer coefficients.

This saturated ground-water flow model was developed using the Boussinesq equation with appropriate initial and boundary conditions. Appropriate boundary conditions include impermeable boundaries, known potential boundaries where an open body of water joins directly to the aquifer or where through a measurement or monitoring program the potential has been determined, and lateral boundaries where only the inflow is known. A significant capability of this numerical formulation of the mathematical model is its ability to handle heterogeneous distributions of the two aquifer properties, hydraulic conductivity and storage coefficient. The output of the model is the transient or steady-state ground-water potential distribution for the area simulated. Streamlines, pathlines, and the associated travel times can also be generated from this predicted distribution of potential.

INPUT DATA

The general kind of field data required, along with the interpretations (generally in a map type format) required to run the model, are shown in the following table. Column 1 shows the general type of data and Column 2 shows the interpretations based on that type of data that must be prepared for input into the model.

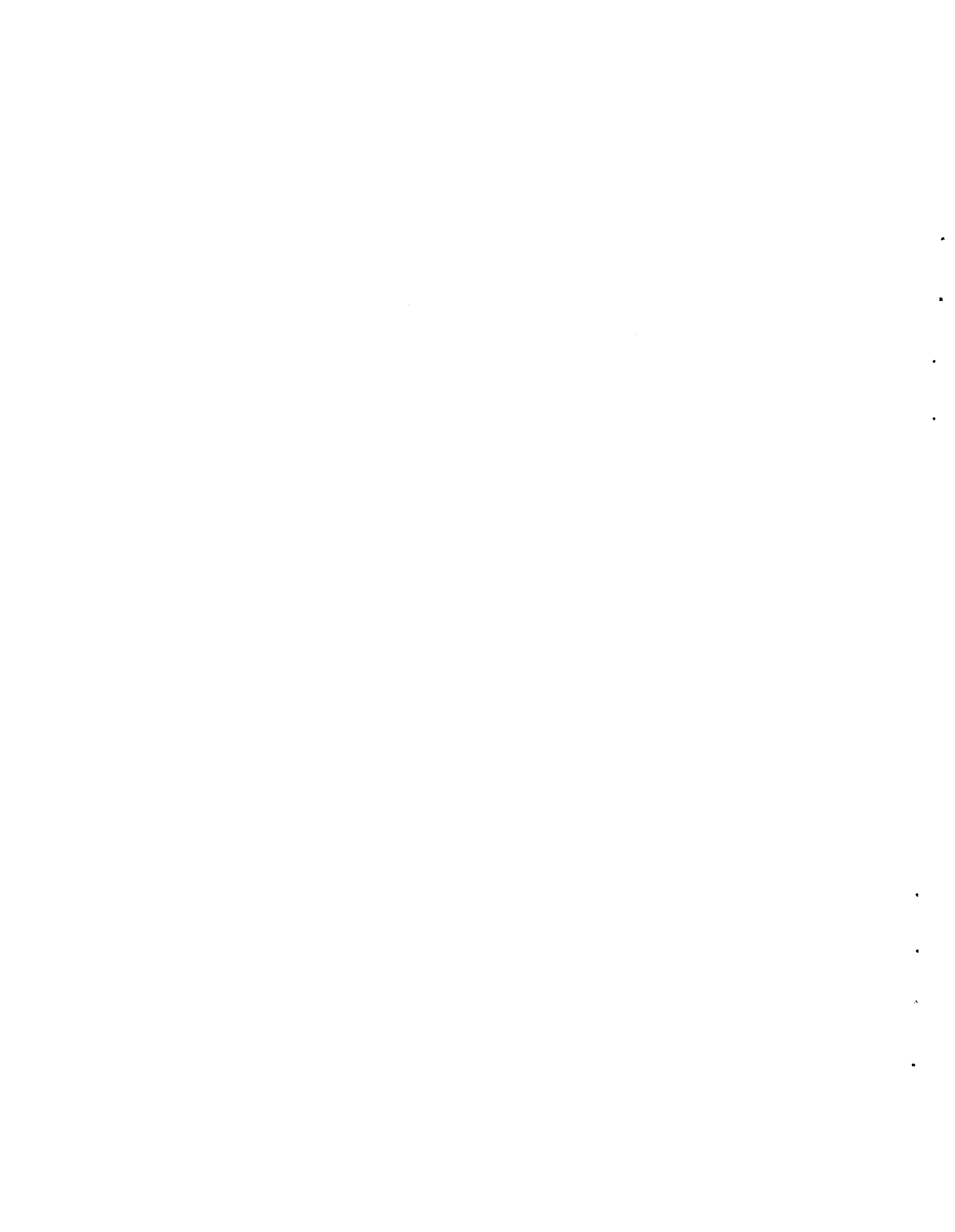
APPLICATIONS

This model has been applied and verified for many hydrologic studies. For example, it accurately modeled changes in ground-water depth on the Hanford Reservation over a 6-year period (Kipp and Reisenauer 1976). The area simulated covered approximately 350 square miles. Sixty-five percent of the area

<u>Type of Data</u>	<u>Interpretations Needed</u>
• Geologic	Aquifer Boundaries <ul style="list-style-type: none"> • Map base and top of aquifer units • Define boundary conditions
• Ground-Water Elevations	Aquifer Potential Maps <ul style="list-style-type: none"> • Interaquifer transfer
• Well Pumping Tests	Aquifer Transmissivity Distributions <ul style="list-style-type: none"> • Storage coefficients
• Recharge and Stress Precipitation Evapotranspiration Well Stress Irrigation	Recharge and Stress Distribution

simulated with the model was within four feet of the measured value after the 6-year simulation and 95 percent was within 15 feet. The average deviation was 4.2 feet.

In another study, the model determined the optimum system for dewatering wells to provide water table suppression (Cole and Foote 1975). This study was conducted for the construction of the Trident submarine dry-dock and involved designing a method of suppressing the head in a coastal artesian aquifer from a plus 40 feet to a minus 68 feet from mean sea level for an extended period of time. Documented data show the matching of the model to a long-term pump test with two different conceptual models of the aquifer configurations. The best match was chosen for the design computation. The calibrated model was able to simulate the drawdown at the end of the pump test with an average error of 2.85 feet.



APPENDIX B

CODE FOR DISRUPTIVE EVENTS

NAME OF CODE: REPOSITORY RELEASE SCENARIO

DESCRIPTION

The Repository Release Scenario Code simulates the geologic and hydrologic systems of the repository site and region during the million-year period following repository closure. The code uses a Monte Carlo technique to generate a large number and wide range of possible geologic evolutionary paths that the geosystem may follow. In generating these paths the model scans and records, for additional study, repository breaches and conditions potentially leading to a breach. A breach is defined as a volumetric flow of ground water through the repository above some threshold value. The various evolutionary paths, their probabilities of occurrence and the breaches or potential breach conditions are used by the AEGIS staff to develop release scenarios.

The simulation portion of the model uses eleven separate submodels. Each of these submodels addresses a geologically related event or process. These include: climate, glaciation, changes in sea level, geomorphic processes, deformation and faulting of repository strata, faulting of basement strata below the repository, hydrology, volcanism, geologic features not detected during site investigation, meteorite impact, and failure of the repository shaft seal. These submodels are a part of a main program that controls the simulation process and handles data input and output. Because of the modular construction of the model, each submodel can easily be replaced with an updated or modified version as new information or developments in the state-of-the-art become available.

Another important aspect of the model is its user-interactive capability. This provides several modes of operational freedom for the user, because the user can readily examine or modify much of the model logic and input data. This capability allows the user to test the effects that modified logic or data will have on the simulation run results. In this way, logic or data that give erroneous results can be quickly identified and corrected.

Because of the enormous amount of data processed and output, the model is being coupled to a sophisticated statistical package. This package will include the Monte Carlo simulation, variance reduction techniques, run time reduction techniques, data analysis techniques, and methods to analyze rare events.

During the one million year simulation run, each submodel is interrogated at predetermined intervals, or time steps. These time steps range from 100 years of simulated time early in the simulation run and increase to as much as 10,000 years late in the run. Progressively increasing time steps are used for two primary reasons. First, the geological process occurrence rates used in the simulation are based largely on the dating of the past geologic events. The accuracy in dating these events decreases as their ages increase. By using short time steps for time periods over which our data are good and progressively longer time steps over periods with less reliable data, computer run time can be decreased dramatically. As an example, if 100-yr time steps are used for the entire one million year simulation run, each submodel must be interrogated 10,000 times. This could result in a computer run time of nearly 2 hours for a single run. By using progressively increasing time steps and other modifications, the run time can be decreased to a few minutes or less. This is very important because several thousand simulation runs may be necessary in the Monte Carlo mode to determine the probable geologic evolutionary paths and possible release scenarios.

The simulation model records everything that occurred during the million-year run into a permanent history file. By examining the history file geoscientists can group similar runs together and identify a few or perhaps several probable evolutionary paths. Those paths that contain breaches or conditions possibly leading to a breach will be flagged for additional study. Geoscientist teams familiar with the repository location will examine each breach and potential breach scenario to determine which of these are most likely to occur. This analysis also allows the geoscientific teams to evaluate the simulation model for logic and input data errors. In this way the model will be continuously refined and updated. Those scenarios determined to be realistic will form the basis for release consequence analyses that involves radionuclide transport and dose models.

The release scenario model can operate in both deterministic and stochastic modes. The deterministic mode allows the user to choose rates and magnitudes of the various geologic events and processes. This mode serves as both a training ground for the user and a testing ground for input data. The stochastic

mode uses pre-established probability distributions for the rates and magnitudes of a wide range of geologic phenomena. In this mode the model uses a Monte Carlo technique to generate a multitude of scenarios that include the common as well as the rare geologic event. This frees the user from having to choose, arbitrarily, discrete values for geologic rates and processes. Also, a wide range of rates and magnitudes can be easily examined to determine their possible effects. In so doing we may find that some geologic events or processes will have no effect on a deeply buried nuclear waste repository.

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APPENDIX C

CODES FOR CONTAMINANT TRANSPORT

NAME OF CODE: MULTICOMPONENT MASS TRANSPORT (MMT)

DESCRIPTION

MMT combines component-porous media interaction models with ground-water flow models, such as VTT, to simulate migration of constituents in ground-water systems. The constituents may be either pollutants (e.g., radionuclides) or major components that are often found in ground water. MMT uses a method called the Discrete-Parcel-Random-Walk (DPRW) technique for modeling mass transport in ground-water systems. The DPRW technique directly simulates the movement of constituents through a ground-water flow field, rather than solving a set of equations that mathematically describe this process.

Two versions of MMT are currently in use: a one-dimensional version (MMT1D) has been used for WISAP-AEGIS preliminary site applications, while a two-dimensional version (MMT2D) has been used for other Hanford site problems (Ahlstrom et al. 1977).

One-Dimensional MMT

MMT1D simulates migration of radionuclides along a one-dimensional flow path. MMT1D simulates both first-order decay of fission and activation products and decay of n-membered decay chains. Radionuclide-geologic media interaction is simulated as retardation that is described by a distribution coefficient (Kd).

Input Data

MMT1D input data include:

- ground-water flow velocity
- longitudinal dispersivity
- flow path length
- dimensions of the stream tube
- nuclide half-lives
- a matrix describing radionuclide chain decay
- soil-to-solution ratio
- porosity
- leach rate information.

Input data for MMT2D include:

- half-lives
- distribution coefficients
- discharge data (rate versus time)
- steady-state or transient x,y velocity fields
- dispersivities for the medium
- aquifer thickness
- boundary conditions
- porosity data.

APPLICATIONS

MMT1D has been or is being used to:

- help evaluate consequences of releases from potential deep geologic nuclear waste repositories
- study alternatives for the ultimate disposition of low-level waste at the Hanford Site
- study consequences of high-level waste tank ruptures at the Hanford Site
- evaluate potential European sites for waste repositories for the International Nuclear Fuel Cycle Evaluation Committee
- evaluate the sensitivity of results to the various input parameters
- evaluate the effects on results of different dispersion mechanisms
- assess the efficacy of performing multi-dimensional simulations by simulating transport along a network of one-dimensional streamtubes generated from VTT or FE3DGW.

The results obtained by MMT1D were compared to the results obtained by an analytical solution (Washburn et al. 1980). It was found that MMT1D and the analytical solution achieved essentially identical results. The analytical solution used has been compared to laboratory experiments. Also, the method used to account for retardation has been shown to model laboratory results adequately (Routson and Serne 1972; Serne et al. 1973).

MMT2D simulates the transport of both pollutants and macro-ions (components commonly found in ground water in relatively high concentrations) in a two-dimensional flow field. Options available with MMT2D include:

- transient convection
- variable dispersion depending on the flow field
- sorption
- variable sorption for nuclides based on the geologic medium and ground-water composition
- first-order radioactive decay
- multiple-layered systems connected with dispersion
- destructive and reflective (no flow) boundary conditions and
- circular-, three-, and four-sided discharge shapes.

The two-dimensional version of MMT has been and is being applied to such problems as:

- tritium migration in the unconfined aquifer at the Hanford reservation for model validation, predicting concentration in a well considered for drinking water, determining the effects of a proposed silvaculture, and determining consequences of restarting fuel reprocessing,
- predicting consequences of a proposed Class A hazardous waste disposal site at Hanford,
- assessing the efficacy of performing multi-dimensional simulations by modeling transport along a network of one-dimensional streamtubes.

It can be considered that this version of MMT has been validated within bounds of error. The approach of the study undertaken to validate MMT was to combine discharge histories and known initial conditions at a given date in order to predict concentrations at a later date in which concentrations are also known. The initial conditions used were Hanford Site tritium concentration patterns as they existed in January 1968, and the final conditions were taken as of January 1976. The resulting computed concentration provided qualitative agreement with the January 1976 data (Ahlstrom et al. 1977).

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APPENDIX D

CODES FOR RADIATION DOSE

NAME OF CODE: KRONIC, SUBDOSA, DACRIN, ARRRG, FOOD, PABLM

DESCRIPTION

The computer programs used for AEGIS to calculate radiation doses to members of the public are a flexible set intended to cover most radionuclide exposure scenarios. Using the various programs, the AEGIS methodology can analyze cases of direct radiation exposure, acute one-time or chronic long-term releases of radionuclides to the atmosphere and acute or chronic releases to surface waters or well water. These various release scenarios relate directly to the AEGIS scenarios for disruptive phenomena, human intrusion, and long-term hydrologic transport.

Atmospheric Dispersion

The concentrations of radionuclides released to the atmosphere, either accidentally or chronically, are calculated using a Gaussian model (Slade 1968). For chronic releases, meteorological data on the joint frequency of occurrence of wind speed, wind direction, and atmospheric stability, and parameters such as release height and plume rise are used for the site and release mechanism involved. The atmospheric concentrations of radionuclides from accidental releases are calculated using the methodology of U.S. Nuclear Regulatory Commission Regulatory Guide 1.3 (USAEC 1974) and of "Meteorology and Atomic Energy" (Slade 1968). For both release types, the vertical dispersion parameters, σ_z , are taken from curves derived from the work of Pasquill (1962) as modified by Gifford (Slade 1968), from Sutton (1953), or from work done at the Hanford Nuclear Reservation (Fuquay et al. 1964). In general, air concentrations are estimated for chronic releases as described above for 16 sectors corresponding to the 16 compass points. Each of these sectors is further divided into ten downwind distances from 0 to 80 km. For chronic releases, horizontal dispersion is determined by the sector boundaries. For acute releases, a horizontal dispersion parameter, σ_y , is found in the same manner as σ_z . For acute releases, concentrations are defined for only one downwind sector, again broken into 10 radial intervals. These models are adequate for sites with fairly level terrain and diffusion in straight lines. Areas with

complicated topography or varying wind patterns will be adequately modeled only for distances close to the release point. These models are used in the computer programs KRONIC (Strengge and Watson 1973), SUBDOSA (Strengge et al. 1975), and DACRIN (Houston et al. 1974; Strengge 1975).

Air Submersion Dose

External exposure results from both gamma and beta radiation emitted from a cloud of radionuclides as they are passing the human receptor. The dose is dependent on the type of radiation, energy, and the spatial distribution of radionuclides in the atmosphere. The computer program KRONIC (Strengge and Watson 1973) is used to calculate air submersion doses from long-term releases to the atmosphere. The beta dose contribution is calculated using a semi-infinite cloud model. This model is used because the range of beta particles in air is short compared to the dimensions of the plume. The gamma dose calculation is more complicated because of the relatively long range of photons in air. To properly determine the gamma contribution, it is necessary to perform a space integration over the plume volume. The gamma dose is calculated as a tissue dose at the body surface, at a depth of 1 cm and at a depth of 5 cm. The beta and gamma doses are reported separately; however, the beta dose and gamma surface dose may be added and reported as a skin dose.

The computer program SUBDOSA (Strengge et al. 1975) is used to calculate air submersion doses from accidental atmospheric releases of radionuclides. SUBDOSA uses the acute release atmospheric dispersion methodology described above, and a space integration similar to that used in KRONIC. Dose results are reported for skin, lens of the eye, total body, and male gonads. Corresponding tissue depths are 0.007, 0.1, 1.0, and 5.0 cm, respectively. Doses are calculated for releases within each of several release time intervals. Up to six time intervals can be allowed and separate radionuclide inventories and atmospheric dispersion conditions can be considered for each time interval.

Limitations of both KRONIC and SUBDOSA are the same as for atmospheric dispersion modeling in general. The bivariate Gaussian plume models are good approximations for straight lines over level terrain. Local variations are difficult to account for.

Inhalation Dose

Radionuclides released to the atmosphere also pose a hazard from inhalation. The computer program used for the analysis of radiation doses from inhalation for AEGIS is DACRIN (Houston et al. 1974; Streng 1975). The program DACRIN uses the model of the ICRP Task Group on Lung Dynamics (1966) to model radionuclide movements in the body. Once radionuclides reach the blood stream, the doses to organs other than the lung are calculated using a single exponential retention function (ICRP 1959).

The model of the respiratory tract adopted by the Task Group on Lung Dynamics forms the general basis for the mathematical models developed to calculate the dose from the inhalation of radionuclides (ICRP 1966). In this model the respiratory tract is divided into three regions, the schematic representation of the respiratory tract used in the development of the mathematical model for the deposition and clearance of inhaled radionuclides is shown in Figure D.1.

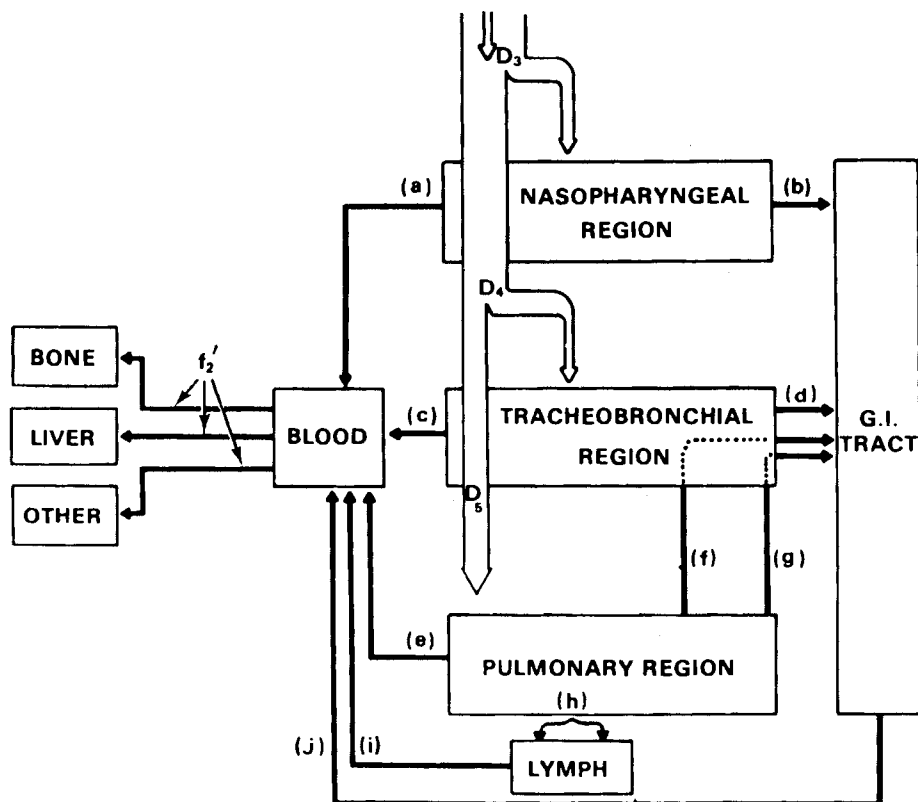


FIGURE D.1. Schematic Diagram of DACRIN Model

Deposition is assumed to vary with the aerodynamic properties of the aerosol distribution and is described by the three parameters D_3 , D_4 , and D_5 . These parameters represent the fraction of the inhaled material, Q_I , initially deposited in the nasopharyngeal (NP), tracheobronchial (TB), and pulmonary (P) regions, respectively. Each of the three regions of deposition are further subdivided into two or more subcompartments. Each subcompartment represents the fraction of material initially in a compartment that is subject to a particular clearance process. This fraction is represented by f_k , where k indicates the clearance pathway. The quantity of material in the TB region, for example, cleared by process (c) is then represented by the product $f_c D_4 Q_I$.

Values of the (f_k) and the clearance half times T_k for each clearance process for the three solubility classes of aerosols used in the code are those suggested by the ICRP (1972). Values of the deposition fractions, D_3 , D_4 , and D_5 , as function of activity median aerodynamic diameter (AMAD) in the form of a graph, have been published (ICRP 1966). Routines to generate these values directly from the AMAD have been included in the code and yield essentially the same values as those presented by the Task Group for the range of particle size distributions considered by that group.

DACRIN also incorporates the ability to calculate atmospheric concentrations using the Gaussian bivariate normal distribution plume model, described above, for either acute or chronic releases. However, externally calculated dispersion factors may be input instead.

Limitations to the DACRIN models include those discussed above as limitations on all atmospheric dispersion models. In addition, data are often unavailable on the physical and chemical characteristics of the inhaled aerosols. Respirable particles are those of sizes below about 10 microns AMAD; particles much larger than this are not readily inhaled. The chemical solubility of the particles is also of importance in calculating lung clearance times. Conservatively low solubilities can be assumed, but this may cause an overestimation of lung dose.

Environmental Contamination Pathways and Doses

When radionuclides are released to the atmosphere or to surface waters, they tend to accumulate in the environment. Radionuclides from the air may

settle on the ground or crops where they can accumulate during the time of the release. If the contamination is in surface waters, it can accumulate in sediments in a lake or river, as well as the water, and also in soils and crops irrigated with the water. These accumulations can result in sources of long-term irradiation of individuals and populations, even from short-lived releases. Sources of dose include direct radiation from contaminated water, sediment, soil and ingestion doses from contaminated drinking water, aquatic food products, terrestrial farm products and farm animals products. For AEGIS, these sources of dose are analyzed using the computer programs ARRRG (Napier et al. 1980a; Soldat, Robinson and Baker 1974), FOOD (Napier et al. 1980a; Baker et al. 1976) and PABLM (Napier et al. 1980b).

The program ARRRG is used to address aquatic exposure pathways. ARRRG can be used to compute internal dose from ingestion of drinking water, fish, other aquatic animals, or aquatic plants, as well as external dose from swimming, boating, and shoreline exposure. Water concentrations of radionuclides are calculated in ARRRG as a function of nuclide release rate, effluent flow rate, and the mixing and dilution in the receiving waters. Mixing and dilution are characterized by a mixing ratio and a reconcentration factor. Formulas for three of the most common reconcentration factors are included in the program. Concentrations in sediments are calculated from the water concentrations, assuming that the water concentration remains constant throughout the release period. Once the release of radionuclides to the water ceases, removal from the sediments is assumed to be by radioactive decay only. Concentrations of radionuclides in aquatic foods are directly related to the concentrations in the water. Equilibrium ratios between the two concentrations, called bioaccumulation factors, are used in ARRRG to calculate the concentrations. These factors implicitly assume immediate equilibrium between the aquatic biota and the contaminating water; equilibrium is reached at the start of the release and ceases at the end of the release. Concentrations of radionuclides in human drinking water are also related to concentrations in surface waters. Radionuclide removal efficiencies for water treatment plants used in ARRRG are based on extensive experience with the processes used for the cities of Richland and Pasco, Washington, downstream of the Hanford Nuclear Reservation on the

Columbia River. Radiation doses calculated from these exposure pathways are based on the simple, single-exponential retention function recommended by the International Commission on Radiological Protection (1959). The doses calculated are a one-year dose, and the 50-year committed dose equivalent from one year of exposure or ingestion.

The program FOOD is used to assess terrestrial exposure pathways. FOOD can be used to compute radiation doses from nine farm or garden crop pathways, five animal product pathways, and external exposure. Radionuclides may be deposited on the ground, crops, or animal forage from either atmospheric deposition or irrigation. The model in FOOD for estimating the transfer of radionuclides (except for ^3H and ^{14}C) from air or irrigation water to plants through both leaves and soil to food products was derived by Soldat and Harr for a study of the potential doses to people from a nuclear power complex (Soldat and Harr 1971). For the atmospheric deposition mechanism, a value of the concentration in air of radionuclides per unit release must be precalculated, as described above, and input to the program. A deposition velocity onto the plant foliage and ground is assumed for the airborne contaminants. Irrigation water concentrations are determined in the program in the same way as for ARRRG. In the absence of specific data for sites where irrigation is used, sprinkler irrigation is assumed, rather than surface irrigation, because the aerial spray produced leads to foliar deposition resulting in higher radionuclide contamination of the plants. For both deposition mechanisms, a plant-to-soil concentration ratio is used to calculate radionuclide concentrations in plants via root uptake. Concentrations of radionuclides in farm animal products, such as milk, eggs, or meat, depends on the animals' consumption of contaminated feed, forage, or water.

For the radionuclides tritium and carbon-14, a special model is used. The concentration of these two nuclides in the hydrogen or carbon content, respectively, of environmental media (soil, plants, or animal products) is assumed to have the same specific activity as in the contaminating medium (air or water). Like ARRRG, FOOD calculates a one-year dose and a 50-year committed dose from one year of exposure.

For some purposes, it is more useful to be able to calculate the total integrated lifetime dose from continuous exposure to changing levels of environmental radionuclides. The computer program PABLM is used by AEGIS to do this. PABLM combines the pathway modeling capabilities of both ARRRG and FOOD. In addition, PABLM allows consideration of changing levels of environmental contamination with time from continuing deposition and radioactive chain decay with daughter ingrowth. PABLM can be used to calculate a 50- or 70-year committed dose from one year of exposure, as well as a 50- or 70-year integrated dose.



APPENDIX E

GUIDE TO AEGIS PUBLICATIONS

GUIDE TO AEGIS PUBLICATIONS

REPORTS

This list of AEGIS publications is broken down by topic. The formal reports, with PNL or BNWL numbers, are available from:

National Technical Information Service
United States Department of Commerce
Springfield, Virginia 22151

Ground-Water Flow and Radionuclide-Transport Analysis

- PNL-2652 C. R. Cole and S. K. Gupta.
A Brief Description of the Three-Dimensional Finite Element Ground-Water Flow Model Adapted for the Waste Isolation Safety Assessment Program.
Pacific Northwest Laboratory.
August 1979.
- PNL-2698 R. W. Wallace.
A Comparison of Evapotranspiration Estimates Using DOE Hanford Climatological Data.
Pacific Northwest Laboratory.
October 1978.
- PNL-2903 P. G. Doctor.
An Evaluation of Kriging Techniques for High Level Radioactive Waste Repository Site Characterization.
Pacific Northwest Laboratory.
January 1979.
- PNL-2939 S. K. Gupta, C. R. Cole and F. W. Bond.
Finite-Element Three-Dimensional Groundwater (FE3DGW) Flow Model--Formulation, Program Listings and Users' Manual
Pacific Northwest Laboratory.
January 1980.
- PNL-2970 W. V. DeMier, M. O. Cloninger,
H. C. Burkholder and P. J. Liddell.
GETOUT - A Computer Program for Predicting Radionuclide Decay Chain Transport Through Geologic Media.
Pacific Northwest Laboratory.
August 1979.

- PNL-3139 D. D. Hostetler, R. J. Serne and
A. Brandstetter.
Status of Sorption Information
Retrieval System.
Pacific Northwest Laboratory.
September 1979.
- PNL-3160 A. E. Reisenauer.
Variable Thickness Transient Groundwater
Flow Model - 3 Volumes.
Pacific Northwest Laboratory.
January 1980.
- PNL-3161 D. R. Friedrichs and R. S. Argo.
CIRMIS Data System - 4 Volumes.
Pacific Northwest Laboratory.
January 1980.
- PNL-3162 R. W. Nelson and J. A. Schur.
PATHS Ground-Water Hydrologic Model.
Pacific Northwest Laboratory.
April 1980.
- PNL-3190 J. F. Washburn, F. E. Kaszeta, S. C. Simmons,
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Multicomponent Mass Transport Model:
A Model for Simulating Migration of
Radionuclides in Ground Water.
Pacific Northwest Laboratory.
June 1980

Radiation Dose Analysis

- BNWL-B-264 D. L. Strenge and E. C. Watson.
KRONIC - A Computer Program for Calculating
Annual Average External Doses from Chronic
Atmospheric Releases of Radionuclides.
Pacific Northwest Laboratory.
June 1973.
- BNWL-B-351 D. L. Strenge, E. C. Watson and J. R. Houston.
SUBDOSIA - A Computer Program for Calculating
External Doses from Accidental Atmospheric
Releases of Radionuclides.
Pacific Northwest Laboratory.
June 1975.

- BNWL-B-389 J. R. Houston, D. L. Strenge and E. C. Watson.
DACRIN - A Computer Program for Calculating
Organ Dose from Acute and Chronic Radionuclide
Inhalation.
Pacific Northwest Laboratory.
December 1974. Reissued April 1976. Errata
December 1977.
- BNWL-B-389 D. L. Strenge.
Supp DACRIN - A Computer Program for Calculating
Organ Dose from Acute and Chronic Radionuclide
Inhalation: Modification for Gastrointestinal
Tract Dose.
Pacific Northwest Laboratory.
February 1975.
- PNL-2636 R. G. Schreckhise.
Model of Long-Term Accumulation of
Radio-Contaminants in Crop Plants.
Pacific Northwest Laboratory.
January 1980.
- PNL-3209 B. A. Napier, W. E. Kennedy, Jr.,
and J. K. Soldat.
PABLM - A Computer Program for
Calculating Accumulated Radiation Dose
from Radionuclides in the Environment.
Pacific Northwest Laboratory.
March 1980.

Release Scenario Analysis

- PNL-2643 J. Greenborg, W. K. Winegardner, P. J. Pelto,
J. W. Voss, J. A. Stottlemyre, I. A. Forbes,
F. B. Fussell and H. C. Burkholder.
Scenario Analysis Methods for Use in
Assessing the Safety of the Geologic
Isolation of Nuclear Waste.
November 1978.
- PNL-2851 B. L. Scott, G. L. Benson, R. A. Craig and
M. A. Harwell.
A Summary of Consultant Input for
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Pacific Northwest Laboratory.
January 1980.

- PNL-2854 S. J. Mara.
Geologic Factors in the Isolation of
Nuclear Waste: Evaluation of Long
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Stanford Research Institute.
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- PNL-2858 S. N. Davis.
Hydrogeologic Effects of Natural Disruptive
Events on Nuclear Waste Repositories.
University of Arizona.
June 1980.
- PNL-2859 M. D. Veatch.
Preliminary Subsurface Hydrologic
Considerations: Columbia Plateau
Physiographic Province.
Seattle, Washington.
April 1980.
- PNL-2862 L. H. Wight.
Feasibility of Computer Interrigation
of Experts of WISAP.
Tera Corporation.
May 1980.
- PNL-2863 C. Bull.
Glaciological Parameters of
Disruptive Event Analysis.
Ohio State University.
April 1980.
- PNL-2864 R. Kehle.
Identifying Suitable "Piercement" Salt
Domes for Nuclear Waste Storage Sites.
Pacific Northwest Laboratory.
August 1980.
- PNL-2882 B. M. Crowe.
Disruptive Event Analysis: Volcanism
and Igneous Intrusion.
Pacific Northwest Laboratory.
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- PNL-2892-1 J. A. Stottlemysre, G. M. Petrie and
G. L. Benson, and J. T. Zellmer.
A Conceptual Simulation Model for Release
Scenario Analysis of a Hypothetical Site
in Columbia Plateau Basalts.(a)
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- PNL-2892-2 G. M. Petrie, J. T. Zellmer, and J. W. Lindberg.
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February 1980.
- PNL-2928 J. A. Stottlemysre, R. W. Wallace, G. L. Benson,
and J. T. Zellmer.
Perspectives on the Geological and Hydrological
Aspects of Long-Term Release Scenario Analysis.
Pacific Northwest Laboratory.
June 1980.

Site Applications

- PNL-2782 J. R. Raymond (Task Leader).
Test Case Release Consequence Analysis for
a Spent Fuel Repository in Bedded Salt.
Bechtel National, Inc., and
Pacific Northwest Laboratory.
January 1980.
- PNL-2955 M. A. Harwell et al.
Reference Site Initial Assessment for
a Salt Dome Repository.(a)
Pacific Northwest Laboratory.
December 1979.
- PNL-3070 C. R. Cole and F. W. Bond.
Comparison of Intera and WISAP
Consequence Model Application.
Pacific Northwest Laboratory.
January 1980.

(a) Available from Project Manager.

WISAP Program Progress

- PNL-2642 H. C. Burkholder, H. H. Greenborg,
J. A. Stottlemire, D. J. Bradley,
J. R. Raymond and R. J. Serne.
Waste Isolation Safety Assessment Program.
Technical Progress Report for FY-77.
Pacific Northwest Laboratory.
April 1979.
- PNL-2874 A. Brandstetter, M. A. Harwell, B. W. Howes,
G. L. Benson, D. J. Bradley, J. R. Raymond,
R. J. Serne, and H. R. Schilling.
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Department of Energy, Washington, DC.
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- BNWL-SA-6100 G. J. Dau.
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- PNL-SA-7184 A. Brandstetter.
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Safety of Radioactive Waste Storage in
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on Migration of Radionuclides in
Crystalline Rocks, Studsvik, Sweden.
11-12 September 1978.
- PNL-SA-7197 J. J. Jacobson (Chairman).
Workshop on Potentially Disruptive Phenomena
for Nuclear Waste Repositories.
Pacific Northwest Laboratory.
27-28 June 1977.
- PNL-SA-7232 J. A. Stottlemire, G. M. Petrie and
M. W. Mullen.
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- PNL-SA-7243 A. Brandstetter and M. A. Harwell.
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- PNL-SA-7468 J. R. Raymond (Chairman).
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- PNL-SA-7480 R. G. Schreckhise.
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- PNL-SA-7872 A. Brandstetter.
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