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Waste Isolation Safety Assessment Program

**Workshop on
Transport Modeling for
Nuclear Waste Repositories**

J. R. Raymond, Chairman

**Seattle, Washington
25-26 July 1977**

**Prepared for
Office of Waste Isolation
under its Contract with the
U.S. Department of Energy**

**Pacific Northwest Laboratory
Operated for the U.S. Department of Energy
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PACIFIC NORTHWEST LABORATORY
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WORKSHOP ON TRANSPORT MODELING
FOR NUCLEAR WASTE REPOSITORIES

J. R. Raymond, Chairman

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INTRODUCTION

Transport Modeling is one task within the Waste Isolation Safety Assessment Program (WISAP) under the National Waste Terminal Storage (NWTs) Program. The NWTs Program is concerned with investigating methods and techniques for using geologic formations to store high-level radioactive wastes from commercial nuclear power reactors. This program is managed for the U.S. Department of Energy by Union Carbide Corporation's Office of Waste Isolation (OWI).

Under OWI sponsorship, Pacific Northwest Laboratory (PNL) is implementing WISAP to develop and demonstrate methods for making comprehensive safety assessments of the long-term isolation of radioactive wastes in geologic media. The Transport Modeling task includes developing methods to describe the transport and impact of radiocontaminants accidentally released from waste repositories; demonstrating the use of these methods; and making the methods and techniques available to the repository managers for application at specific sites. The initial focus of this task will be a system of models for estimating the consequences of intrusive events that may lead to a water transport pathway for contaminants through the geologic media to points of potential human uptake. Available hydrologic, transport and dose models will be adapted and/or extended to implement this task.

The workshop on Transport Modeling for the Waste Isolation Safety Assessment Program was held at the Battelle Seattle Research Center on 25 and 26 July 1977.

The objectives of the workshop were to: 1) discuss needs and criteria for the models, 2) obtain critiques of proposed model systems from experts in the field, and 3) obtain ideas for making models more useful to the safety assessment program.

WORKSHOP PROCEEDINGS

PARTICIPANTS

Eighteen experts in the fields of hydrologic (ground water) and transport modeling participated in the workshop. In addition, eight persons attended as observers (members of OWI, ERDA, Coal-Review Group, PNL Internal Review Committee, etc.). Six PNL staff members gave presentations to provide information on WISAP and its respective tasks. Also, the workshop participants were provided with a Source Book that contained background data on WISAP and descriptive summaries for hydrologic, transport and dose models.

MODELING ASSUMPTIONS

The following assumptions were proposed for discussion concerning hydrologic and transport modeling for the WISAP program:

1. Existing technology will be used - there will be no extensive research efforts. However, some development work will be required to revise and/or adapt models and codes. Neither funding nor time constraints permit development of totally new technology. Also it is felt that, for the most part, models are available that can adequately address the problem.
2. No ground water or surface water will be present initially at waste isolation repository sites.
3. Exposure of the waste to water and development of hydrologic systems will be due to "disruptive events."
4. Only far-field and long-term situations will be considered.
5. Only saturated flow systems will be modeled.
6. The flow system will be treated as a continuum.

7. Model input data will be general and imprecise, for the most part.
8. Contaminants of concern will be present in the ground water in trace amounts.
9. Diffusion of solid waste through a solid medium or a dry porous medium will not be significant, even over long time periods.

Changes were recommended for several of the assumptions. It was suggested that assumption No. 2 be deleted as it is ambiguous, probably inaccurate, and actually affects only the time frame and not the methods of analysis. Participants felt that assumption No. 3 should be modified to read, "Exposure of the waste to water will be due to disruptive events." Also, in assumption 4, the consensus was that "far-field" should be deleted, as we may have to evaluate near-field effects. It was agreed that the material leached from the waste form will be in trace amounts chemically in the ground water, but this may result in high radioactivity. It would be better to add "chemically" before the phrase "trace amounts."

Participants felt that criteria No. 2 should be modified to read, "The model system will be able to utilize input data from geohydrologic systems that will vary from simple to complex. Also, the suggestion was made that, in No. 3, the transport codes will consider solute/solute interactions. Furthermore, a recommendation was made that expansion and amplification of the assumptions and criteria be made to make clearer definitions.

The following modeling criteria and requirements were proposed:

1. The modeling approach must be applicable to a number of specific sites having diverse geology and hydrology.
2. The model system will be able to utilize input data that will vary from simple to complex.
3. Transport codes will consider solute/media interactions and radioactive decay and growth.
4. The modeling approach must predict the arrival time and concentrations of contaminants at points of uptake.
5. Transport travel times of up to 10^6 years must be addressed.

STATE OF THE ART

The nature of the location of waste repository sites and the ambiguities of the radioactive release scenarios will usually provide only general information on input parameters for hydrologic and transport models (permeability, porosity, coefficient of storage, hydraulic gradient, aquifer base level, distribution coefficients, etc.). Also, there are wide variations in the "state-of-the-art" for hydrologic modeling, transport modeling, and dose modeling. The technology is more advanced for modeling of fluid flow in complex groundwater systems than for modeling contaminant transport in those systems. Likewise, dose modeling requires more simplifying assumptions and is less rigorous than hydrologic or transport modeling. Recent compilations and assessments of modeling technology show that there are numerous hydrologic models available to assess a wide variety of groundwater flow systems from the very simple, one-dimensional, homogeneous, isotropic, single-layer, steady-state, saturated flow conditions to the most complex three-dimensional, heterogeneous, anisotropic, multilayer, transient, partially-saturated flow case. There are fewer groundwater transport models available, but they also span a wide range of simple to complex conditions. Only one environmental consequence model set (dose model) considers radioactive dose (both external exposure and ingestion exposure) from the water pathway.

WISAP MODELING APPROACH

The argument could be made that only a simplistic modeling system should be implemented for WISAP since input data probably will be inaccurate and of a general nature and there is no need for a complex hydrologic model to provide input for simplistic transport and dose models. This argument has some validity, but there is also the necessity of providing assessment of more complex systems when and if adequate data become available. Also, at times, there is the requirement to demonstrate that "best practicable technology" was used or at least available and considered. Therefore, it is intended that the modeling system developed will be capable of assessing a

wide variety of cases ranging from conditions where only minimal data are available on hydrologic, transport, and dose parameters to areas where detailed input information will be derived.

A system was proposed for WISAP that will consist of four levels of complexity with each level having a hydrologic model, a transport model, and a dose model. The hydrologic model defines water flow paths and travel times from input data provided by repository disruptive event analysis. The transport model utilizes the output from the hydrologic model and radioactive release source terms to describe the movement of the contaminants through the geosphere and provides rates and concentration of radioactive release to the biosphere (in this case, to a surface-water body). This output then serves as an input to the dose model which provides the environmental dose assessment of the radioactive release. The models will be adapted to operate in a coupled fashion whenever possible. Although selected models will be utilized for demonstration, it is important to recognize that there may be several model systems that may be useful and applicable, and the intent of the model implementation is to demonstrate level of technology.

First Modeling Level

The first level of the proposed system will be the simplest. The hydrologic model will be an analytical solution of the Darcy equation (or other steady-state flow equations) to derive groundwater velocities from disruptive events for input to the transport model. The first level transport model proposed was GETOUT.¹ The GETOUT model assumes that at some arbitrary time after the waste is deposited, the contents of the site are dissolved at a specified constant rate into an underground water stream. The water stream flows at constant velocity through a homogeneous, one-dimensional column of the geologic medium and discharges to a surface-water body. The dissolved radionuclides are assumed to be in sorption equilibrium at all points in the geologic medium. Radioactive decay (including chain decay of the actinides) is modeled both at the disposal site and during migration through the geologic medium. Trace

concentrations of the dissolved nuclides are assumed, and as a result the adsorption equilibrium constants are independent of concentration. A constant axial dispersion coefficient is also assumed. This model is applicable to particulate and fractured media provided the necessary input data are obtained properly and can be applied to the relevant input parameters.

The proposed first-level dose model was ARRRG/FOOD.^{2,3} This set of computer codes was developed for calculation of annual radiation dose and long-term commitments to the total body and selected organs of individuals and population groups from both internal and external sources of radiation. ARRRG calculates annual individual and population doses resulting from radionuclides released with liquid effluents. Presently, nine exposure pathways may be selected by the operator; consumption of fish, crustacea, molluscs, algae, and drinking water; and direct external radiation from the shoreline, water immersion (swimming) and water surface (boating). Doses are calculated for skin (external only), total body, GI-LLI (gastro-intestinal tract, lower large intestine), thyroid, bone, liver, lung, and kidney. Individual contributions to dose by nuclide and by pathway are output.

FOOD calculates annual individual doses from the consumption of garden foods and animal products contaminated from air deposition or water (sprinkler irrigated). Presently, 14 food types may be selected. GETOUT, ARRRG, and FOOD have already been applied as an integrated system to estimate the dose consequences of nuclide transport following a hypothetical failure at a nuclear waste repository.⁴ These codes are written in the Computer Sciences Corporation's version of CSTS Basic for interactive use from a remote terminal. This system operates on a UNIVAC 1108 computer. The interactive mode enhances the flexibility of varying data parameters and shortens the turnaround time required to obtain results.

Second Modeling Level

The second level of the proposed system will utilize somewhat more detailed hydrologic data. The hydrologic model proposed was an idealized

analytic or hybrid analytic/numerical code that will provide for solution of groundwater potential distribution and flow pathlines. The PATHS computer program⁵ provides such a model. PATHS is a two-dimensional analysis tool for determining saturated groundwater arrival times at a river type outflow boundary. The code was purposely designed to provide a realistic balance between model complexity and the limited input data usually available. Accordingly, the basis of the code is an idealized, two-dimensional analytical solution for the groundwater potential distribution. From the potential distribution, the pathline differential equations are numerically solved by the code to give the paths of the fluid particles and their advance with time along the paths toward the outflow boundary. The program uses an interactive Basic front end which leads the user through the program input, requesting the data needed and helping the user to select the necessary control parameters. After the input is completed, the Basic part of the program automatically submits a "batch" job, thereby capitalizing on the economy available during heavy computing while solving the simultaneous equations. The results are available as: 1) summary tables obtained interactively, 2) detailed computer printouts when desired, or 3) as Calcomp plots, if that option is selected.

GETOUT was also proposed for the second-level transport model and ARRRG/FOOD was proposed for the dose model.

Third Modeling Level

The third level of the proposed system is more complex (in the hydrologic evaluation) and will provide for more rigorous evaluation of the groundwater systems where such evaluation is justified by the input data. Either the free-surface flow approach or the Boussinesq approximation method can be used to accurately model complex two-dimensional, heterogeneous, anisotropic, transient, saturated, groundwater flow systems. The Variable Thickness Transient Flow Model (VTT)⁶ was proposed for this use. The model originated from a standard finite difference Boussinesq formulation, but has been enhanced as various problems have been solved to date. It has multi-aquifer capability with variable thickness features for the unconfined strata and can solve both transient and steady-state problems. More

detailed solution at a finer difference grid spacing is possible by a sequential solution process wherein the results of a large region simulation are used as boundary conditions for a smaller region. The model has flexible interactive evaluation capability. Part of the interactive flexibility of VTT centers upon extensive input assistance and checking features to assure that the problem is free of input inconsistencies. The extensive output capabilities are most useful in effectively demonstrating the solution process for complex problems.

The third level transport model proposed was GETOUT, although investigation will be made to: 1) determine if one of the more complex numerical transport models, such as the Multicomponent Mass Transport (MMT) Model⁷ can be adapted to include consideration of radioactive chain decay, and 2) determine if it is practical to use a complex numerical model over the long time periods of interest to geologic isolation safety assessments.

The only applicable dose model was the ARRRG/FOOD set proposed for levels one and two, above.

Fourth Modeling Level

The proposed fourth level of the system would contain the most advanced and complex model technology available. There are several hydrologic models available. One example is the DAVIS FE Model⁸ which is a model that considers saturated groundwater flow in three dimensions, with both the fluid and porous material considered compressible. The time dependence arising from compressibilities is considered through a backward difference, and the spatial discretion is through finite elements. Three-dimensional isoparametric elements are used that can be deformed in any of the three coordinate directions. The spatial basis functions for the isoparametric shapes along any element edge may be either linear, quadratic, or cubic in functional form. Such functional forms are incorporated by inserting node points along the element edge, i.e., the two end points are used for the linear form. Adding a node at the center provides the quadratic variation, and the cubic is obtained through adding internal nodes at the one-third points along the element side. This procedure allows flexibility,

particularly in satisfying irregular boundary conditions, yet maintains the advantages of using the simpler Chapue basis functions for the potential or head representation.

Also, the VCHFLD (variational model for calculating transport and dispersion of chemical constituents) and DWDM (deep well disposal model) models will be investigated to determine applicability for fourth-level flow and transport models. Review of model technology has not identified comparable dose models for use in conjunction with the three-dimensional flow and transport models.

RECOMMENDATIONS

Discussion revolved around the need for various levels of complexity for the hydrologic and transport models. The consensus seemed to be that the second modeling level might be deleted, but the general concept of having multiple levels of model technology available to evaluate simple to complex systems seemed to be accepted.

The various models that appeared applicable to the different levels were discussed using the Source Book table for a range of models useful in waste isolation assessment. Several additional models were added to the table.

Recommendations were made that the modeling efforts would be more convincing if transport involved in events of the past, such as the Oklo natural reactor, could be modeled. This exercise could serve as a verification study. Also some observers felt that the modelers should not become so involved with the fine structure and detail, that they forget to look at the broad picture, which will be adequate for realistic evaluations.

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