A GENERALIZED WASTE PACKAGE CONTAINMENT MODEL

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ABSTRACT

The U.S. Department of Energy (DOE) is developing a performance assessment strategy to demonstrate compliance with standards and technical requirements of the Environmental Protection Agency (EPA) and the Nuclear Regulatory Commission (NRC) for the permanent disposal of high-level nuclear wastes in geologic repositories. One aspect of this strategy is the development of a unified performance model of the entire geologic repository system. Details of a generalized waste package containment (WPC) model and its relationship with other components of an overall repository model are presented in this paper. The WPC model provides stochastically determined estimates of the distributions of times-to-failure of the barriers of a waste package by various corrosion mechanisms and degradation processes. The model consists of a series of modules which employ various combinations of stochastic (probabilistic) and mechanistic process models, and which are individually designed to reflect the current state of knowledge. The WPC model is designed not only to take account of various site-specific conditions and processes, but also to deal with a wide range of site, repository, and waste package configurations.

INTRODUCTION

The U.S. Department of Energy (DOE) is developing a performance assessment strategy to demonstrate compliance with standards and technical requirements of the Environmental Protection Agency (EPA) and Nuclear Regulatory Commission (NRC) for the permanent disposal of high-level nuclear wastes.[1,2,3] This strategy involves the use of performance models to estimate the containment times and the eventual release rates of radionuclides from waste packages emplaced in a geologic repository, and steps to develop a unified and comprehensive geological repository performance model have recently been undertaken.[4,5]

In order to fulfill the performance assessment function, any comprehensive model which is developed must be

- general, in order to permit release estimates to be computed for a wide range of repository designs and geologic/geochemical environments, and
- flexible, in order to take into account various site-specific conditions and processes.

A successful model must include all the important processes which either individually or jointly affect radionuclide containment or release. Further, the model should be designed to provide "expected" or "realistic" estimates of release (not just "worst case" estimates), together with estimates of uncertainty which take account of current information about the processes, models and input values used to determine the release. Selected aspects of a unified performance model, with emphasis upon a stochastically-driven waste package containment model, are discussed in this paper.

THE SOURCE-TERM MODEL

Shown in Fig. 1 are the two major components of a geological repository performance model, a Repository Source-Term (AREST) model and a Contaminant Transport model. The Source-Term model is further broken down into three components:

- a Waste Package Containment model,
- a Waste Package Release model,
- an Engineered System Release model.

The Waste Package Containment (WPC) model simulates those corrosion processes and degradation mechanisms (e.g., mechanical stresses) which ultimately result in failure of a waste package to exclude groundwater from contact with the waste form. Upon penetration of the waste package by groundwater, the Waste Package Release model (WPR) simulates the release of radionuclides and their migration outward through corroded openings. Finally, the Engineered System Release (ESR) model integrates the releases from individual waste packages to provide the (distribution of) total release from the repository as a function of time and space. The three models operate sequentially, with output from one model serving as input to the succeeding one.[4,5]

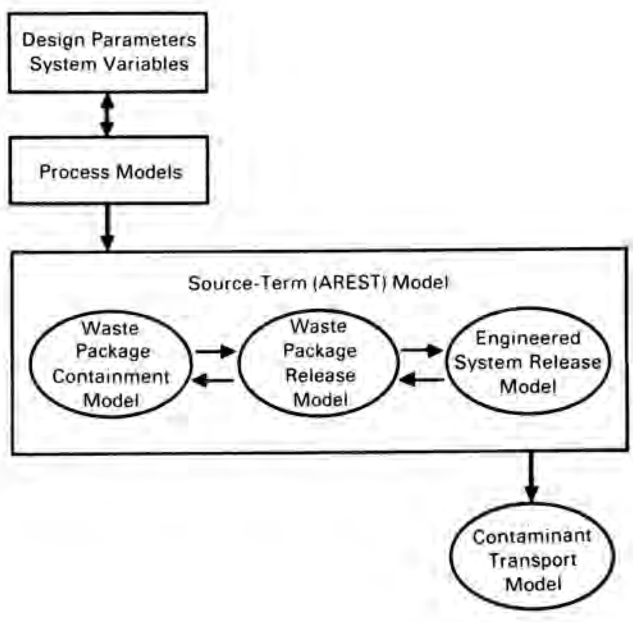

Fig. 1. The Geologic Repository Performance Model

Considerable information is required to drive the source-term model shown in Fig. 1. Design parameters and system variables which describe the repository, the site and the waste package are required, as are models of important physical and chemical processes.

Table I contains lists of parameters and variables which might be used to describe the repository, the site and the waste package. The lists, presented here for the sake of discussion, are neither definitive nor exhaustive. Table I has been compiled from a variety of sources, however, so it does illustrate the range of factors which are being considered by performance assessment modelers.[3,6-9] Those descriptors (or inputs) from Table I whose values can either be controlled or fixed with negligible uncertainty are referred to as design parameters. Inputs of a stochastic nature are referred to as system variables; system variables include those inputs whose values are not precisely known or which are subject to significant variability under a fixed set of (initial) conditions. The composition of the canister is regarded as a design parameter, for example, whereas the temperature of its contents at the time of emplacement is a system variable. Despite its utility, the distinction between design parameters and system variables may be difficult to make in practice (as in the case of "type of waste form", for example).

For any potential repository, site and waste package configuration, it will be necessary to assign a value to each applicable design parameter and system variable. This can be accomplished for design parameters by a means of a list of values from which an appropriate value is selected. For system variables, an appropriate distribution is first selected from a list of distributions and the input value is then simulated from the selected distribution. The list of distributions may include fixed values in the form of point (degenerate) distributions.

Table II contains a list of models of physical and chemical processes which NRC currently considers to be important for waste package performance assessment.[3] While models for the specified processes should be included in the development of any performance assessment model, the use of models for other processes is not precluded. Site-specific conditions will be modeled insofar as possible by changing the values of parameters in a general process model, but it is conceivable that several process models will be required to encompass a sufficiently wide range of site-specific conditions (the corrosion rates of low-carbon steel in salt and basalt may not be governed by the same equation, for example). By simulating the values of process model parameters from pre-assigned probability distributions, it will be possible to incorporate uncertainty into the process model, and ultimately into the geological repository performance model.

TABLE I

Repository, Site and Waste Package Descriptors

Repository Descriptors

Host material (basalt, granite, salt, tuff)
Areal dimensions
Distance between adjacent canisters
Number of canisters
  (or capacity, i.e., number of
  canisters times canister capacity)
Number of canisters per room (if applicable)
Bore hole radius
Bore hole orientation (e.g., degrees from vertical)
Thickness of disturbed rock zone

Site Descriptors

Host Material
- Density
- Porosity, Permeability
- Effective porosity
- Adsorptive properties
- Kd, or related sorption coefficients
- Shortest path to accessible environment
- Temperature
- Thermal conductivity coefficient

Fluid/Groundwater
- Eh (redox potential)
- pH
- Pressure
- Flow rate - near field
- Flow rate - far field
- Resaturation rate (if applicable)
- Brine migration rate (if applicable)
- Diffusion coefficients
- Hydraulic conductivity
- Hydraulic gradient
- Advective properties
- Concentrations of complexants (F^-, CO_3^{-2}, S^{-2}, etc.)
- Additional variables required to drive corrosion models

Waste Package Descriptors

Packing Material
- Type (e.g., basalt-bentonite, air)
- Composition (e.g., 25% basalt - 75% bentonite)
- Thickness
- Density
- Porosity, Permeability
- Effective porosity
- Diffusion coefficient
- Hydraulic conductivity
- Hydraulic gradient
- Kd, or related sorption coefficients
- Adsorptive properties
- Thermal conductivity coefficient

Canister/Container/Overpack
- Composition (stainless steel, low-carbon steel, etc.)
- Dimensions (length, outer diameter, inner diameter, etc.)
- Wall thickness
- Corrosion allowance
- Stress allowance
- Capacity
- Time of emplacement
- Net weight
- Thermal conductivity coefficient

Waste Form
- Type (spent fuel, borosilicate glass, etc.)
- Composition
- Dimensions
- Cladding thickness (if applicable)
- Initial thermal output
- Initial temperature at centerline
- Initial (γ) radiation level
- List of "important" radionuclides and the inventory, half-life, specific activity, solubility, and adsorptive coefficients for each

TABLE II

Examples of Important Performance Models (Source: Reference 3)

Model (Dependent Variables)	Function of:	Corresponding AREST Submodel
Temperature	Time, Location	WPC
Heat Source	Time	WPC
Radiation	Time, Location	WPC
Groundwater Flow Model	Time, Temperature	ESR
Water Chemistry (pH, Eh, salt concentrations, etc.)	Time, Temperature, Flow Rate, Radiation	WPC
Corrosion (uniform, pitting, etc.)	Temperature, Water Chemistry, Radiation	WPC
Mechanical Failure	Stresses	WPC
Leach (release rates of radionuclides)	Time, Temperature, Water Chemistry	WPR
Buffer Transport (radionuclide concentrations)	Time, Temperature, Water Chemistry and Water Flow, Radiation	WPR

THE WASTE PACKAGE CONTAINMENT MODEL

The WPC model is designed to simulate, as realistically as the current state of knowledge allows, the performance of a typical waste package under repository conditions. The waste package is defined as "penetrated" at the time physical containment is lost and the possibility for release of radionuclides exists. The basic output of the WPC model is a series of "penetration times" for individual waste packages; these times are used, in turn, to estimate the distribution of waste package penetration times for the repository. Other outputs include the values of variables, at the time of penetration, which are required by the WPR model to estimate release rates and chemical reaction times.

Model Structure

The basic logic and modular structure of the WPC model are revealed in Fig. 2, where steps in the simulation of an individual waste package are shown. The model contains modules for simulating steam corrosion and other processes which lead to failure of the canister and (if applicable) the Zircaloy barrier.* An individual metallic barrier of the waste package is defined as "failed" at the time its net thickness at some locale becomes zero due to corrosion or rupture, i.e., at the time it ceases to perform as a physical barrier to groundwater intrusion. In cases such as the Canister Performance module, where several corrosion processes operate simultaneously (see Fig. 3), the processes are simulated until failure is indicated for at least one. The time-to-failure for the canister is then taken to be the minimum of the indicated failure times for all the process being simulated.

Upon failure of a barrier, provision is made to model a period of "aperture growth." Aperture growth is defined as the (post-failure) change in the total cross-sectional area of local failed regions. The aperture growth models can also account for changes in radionuclide release and corrosion rates resulting from attention of groundwater access to the waste form and the effects of corrosion products precipitated at the corroding surfaces. A "worse case" model would specify that the area of failure becomes maximal at the time of penetration.

*For glass waste forms, appropriate corrosion models for the proposed stainless steel "pour containers" would be used in place of the Zircaloy module.

Simulation of each waste package proceeds from one module to the next in the order indicated in Fig. 2. The Steam Corrosion module, if applicable, operates until changing environmental conditions (temperature, pressure) result in the condensation of steam to liquid water. At this time, the Canister Performance Model is activated. Likewise, the Canister Aperture Growth model and (if applicable) the Zircaloy Barrier Performance models are initiated at the time of canister failure. The Zircaloy barrier performance model allows for the possibility that the cladding is in a state of failure initially, in which case $T_4 = T_3$ (see Fig. 2).

The hierarchical structure of the model is illustrated in Figs. 2 and 3; the latter shows an additional level of detail for the Canister Performance module. If corrosion mechanisms other than those shown are found to be important, provision is made for models of these mechanisms to be added. Conversely, if a particular corrosion model is found to be inapplicable, it is simply bypassed during simulation.

One example of a rate equation is that presented by Westerman, et al.[10] for uniform corrosion of low-carbon steel in a salt environment. The authors use laboratory data to derive an equation which relates uniform penetration rate to temperature, radiation dose rate, flow rate and other system variables. When available, deterministic models such as this uniform corrosion model will be used in the source-term model. Uncertainty can be introduced by assigning distributions to model input parameters on the basis of best-available information from site characterization and design studies. Where suitable mechanistic models are unavailable, probability models (distributions) can be used instead.[9,11] If a particular process (e.g., uniform corrosion) cannot be modeled under all conditions of interest by changing inputs to a single general model, it will be necessary to compile a list (menu) of specific models from which an appropriate one can be chosen.

Model Operation

The WPC model, as conceived, simulates the time-to-penetration of one waste package at a time, until penetration times have been simulated for all the waste packages in the repository. First, the values of repository design parameters and other non-stochastic descriptors are fixed. Then,

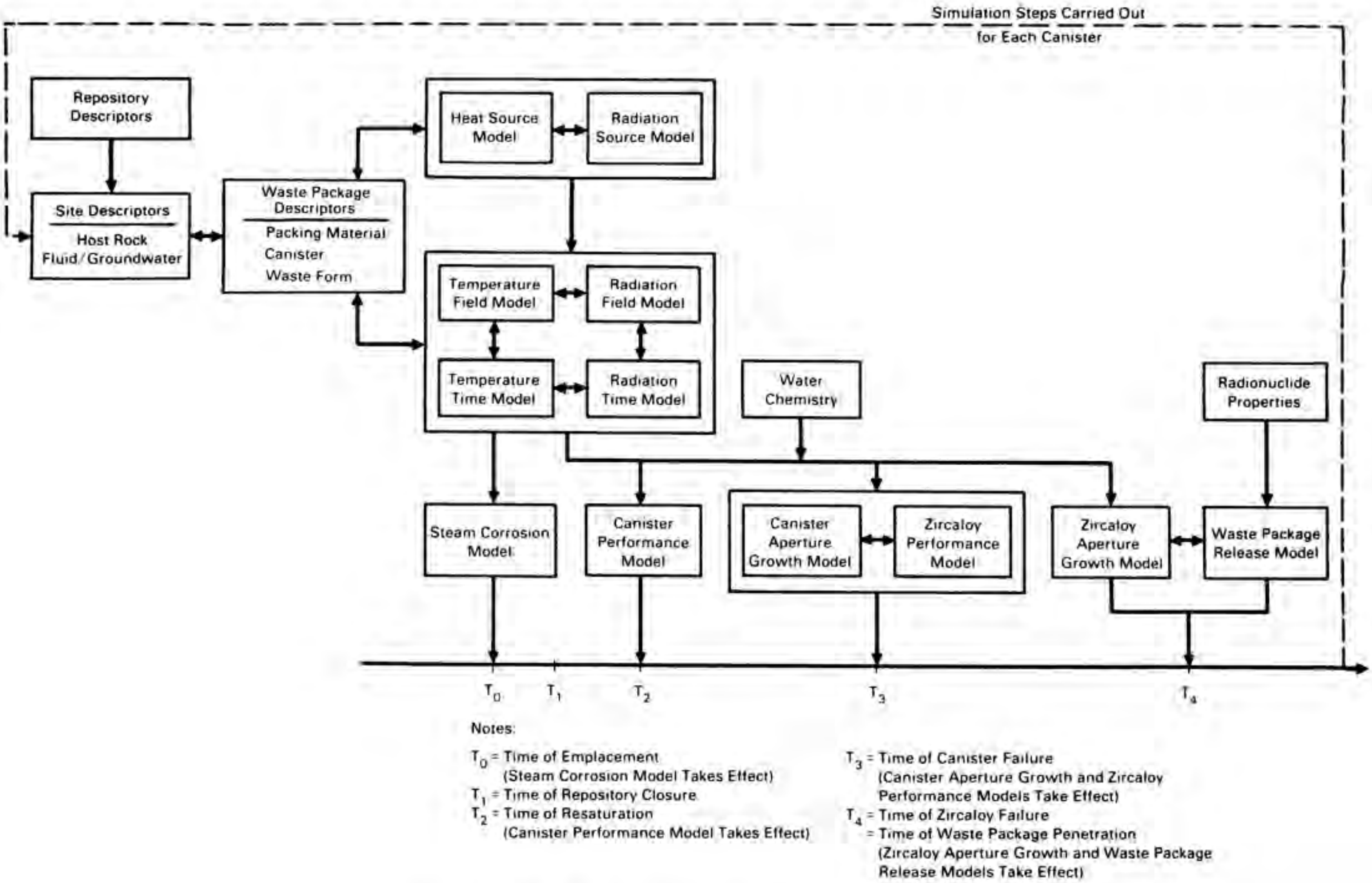

Fig. 2. The Waste Package Containment Model

simulation for each waste package proceeds through the following steps:

- For the specified repository, site and waste package configuration, appropriate probability models are selected to describe (the initial distributions of) system variables. Initial values of system variables are then simulated from specified input distributions.
- After the initial values of system variables are established, the waste package is simulated until it fails. Simulation involves exercising the Steam Corrosion module, the Canister Performance module, and the Canister Aperture Growth and Zircaloy Barrier Performance models. Modules for processes which are inapplicable (e.g., steam corrosion when salt is the host material) are bypassed.
- The time-to-penetration is recorded, together with other information which is required as input to the WPR model.
- The preceding steps are repeated for each waste package.

The values of design parameters, once established, are fixed throughout simulation of an entire repository. Values of system variables, on the other hand, are changed via simulation for each waste package. Although values of design parameters are fixed throughout a simulation, any implementation of the proposed model should allow them to be readily changed. By making it easy to change not only the distributions of system variables, but also the values of design parameters, the model can be made flexible enough for use under a wide range of site, repository and waste package configurations.

Model Features

The Waste Package Containment model proposed in this paper has several features which make it attractive for performance assessment. Its modular structure gives the model flexibility and a wide range of applicability, both of which can be exploited to increase "realism." As new information becomes available, new modules can be added or affected modules can be modified without the need for a full-scale revision of the overall model. Moreover, because of its modular structure, the model can incorporate a mixture of stochastic (probabilistic) and mechanistic components. Stochastic models can be used where mechanistic models are unavailable. Where mechanistic models are available, uncertainty can be incorporated into them via model inputs. Probability distributions for system variables and inputs to mechanistic models are based upon experimental data to the extent that such data exist. Where experimental data are inadequate, probability distributions are established with the aid of best-available information.

By treating design parameters as input variables (so their initial values can easily be changed), it will be possible to set up configurations which describe a wide variety of repository designs and/or geologic environments. While such capability is clearly important for performance assessment, its utility for the comparison of potential repository

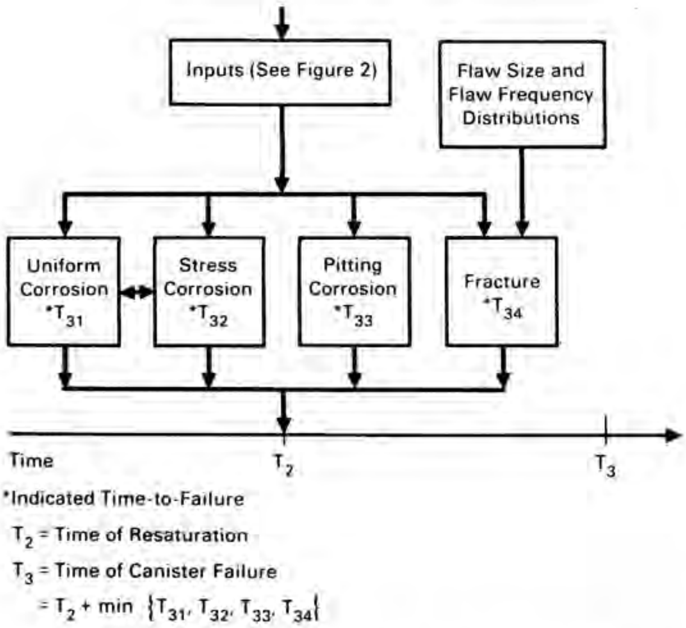

Fig. 3. Detail of Canister Performance Model

designs is also obvious. Similarly, lists of input distributions for system variables and, if necessary, lists of process models as well, are used to make the model general enough to encompass the expected range of repository designs and site conditions.

Models of spatial and temporal variation in important variables such as temperature and radiation also serve to increase realism. In this regard, supplemental output from the components of the source-term model may prove helpful for understanding the factors which affect waste package performance. As one example, a breakdown by barrier and corrosion mechanism of the times-to-penetration for simulated waste packages may provide some insight concerning which mechanisms have the greatest effect.

SUMMARY

The availability of a reliable waste package containment model is essential to the success of DOE efforts to develop a unified geologic repository system performance model. A general waste package containment model is proposed in this paper. The primary output of the model is series of times-to-penetration by groundwater of individual waste packages under a particular set of repository and site conditions. These times are used to estimate total release from the repository. The WPC model, although general, is flexible enough to take account of site-specific conditions and processes. The model contains both mechanistic and probabilistic components, with the mixture of the two being determined by the current state of knowledge about the particular process being modeled. Possible inputs to the model are listed in Table I and important component models are listed in Table II.

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REFERENCES

1. U.S. Environmental Protection Agency, Federal Register 47 (250: 58196-58206 (Proposed 40 CFR 191), December 1982.

2. U.S. Nuclear Regulatory Commission, 10 CFR 60, Federal Register 48 (120): 28194-28229, June 1983.

3. U.S. Nuclear Regulatory Commission, "Draft Generic Technical Position on Waste Package Reliability," October 1984.

4. D. H. ALEXANDER, M. J. APTED, A. M. LIEBETRAU, A.E. VAN LUIK, R. E. WILLIFORD, and P. G. DOCTOR, "Conceptual Model for Deriving the Repository Source Term," in Scientific Basis for Nuclear Waste Management VIII, eds. C. Jantzen, J. Stone and R. Ewing. Materials Research Society Proceedings, 1985.

5. M. J. APTED, D. H. ALEXANDER, A. M. LIEBETRAU, A. E. VAN LUIK, R. E. WILLIFORD, and P. G. DOCTOR, "A Conceptual Model for Repository Source-Term Evaluation," presented at the DOE/OECD Workshop on Repository Source-Term Models, Albuquerque, November 13, 1984.

6. W. V. HARPER and G. E. RAINES, "Probabilistic Analysis of Human Intrusion in a High Level Nuclear Waste Repository in Salt Using Draft EPA Assumptions," Battelle Memorial Institute Office of Nuclear Waste Isolation, Columbus, Ohio, 1984.

7. R. B. LYON, "Environmental Safety Assessment for Nuclear Waste Disposal - The Canadian Approach," presented at the Symposium on Waste Management, Tucson, February 1981.

8. R. B. LYON, "Nuclear Waste Disposal: The Interface Between Performance Assessment and Research," in Scientific Basis for Nuclear Waste Management, Vol. 16, ed. S. V. Topp, Elsevier Science Publishing Co., New York, 1982.

9. B. SAGAR, P. W. ESLINGER and R. G. BACA, "Probabilistic Modeling of Radionuclide Release at the Waste Package Subsystem Boundary of a Repository in Basalt," SD-BWI-TA-012, Rockwell Hanford Operations, Richland, Washington, December 1984.

10. R. E. WESTERMAN, J. L. NELSON, S. G. PITMAN, W. L. KUHN, S. J. BASHAM and D. P. MOAK, "Evaluation of Iron-Base Materials for Waste Package Containers in a Salt Repository," in Scientific Basis for Nuclear Waste Management VII, ed. G. L. McVay, pp. 427-436, North Holland, New York, 1984.

11. M. S. CHU and C. L. AXNESS, "A Comparison Study of Different Source Models for High-Level Waste," presented at the Symposium on Waste Management, Tucson, March 1984.