AREST: A PROBABILISTIC SOURCE-TERM CODE FOR WASTE PACKAGE PERFORMANCE ANALYSIS

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ABSTRACT

The engineered barrier system (EBS) is the first of several man-made and natural barriers to the release and migration of radioactive wastes from a geologic repository to the accessible environment. The Analytical Repository Source-Term (AREST) code has been developed to provide a quantitative assessment of the performance of the EBS and its individual barriers relative to the regulatory requirements for the isolation of nuclear wastes. The AREST code can therefore serve as the source-term component of a code (or codes) designed to evaluate the performance of the entire geologic repository system.

The AREST code integrates mechanistic models of chemical and physical processes that affect radionuclide release into a unified probabilistic framework. The code initially simulates those corrosion processes that ultimately result in the failure of the metallic barriers of a waste package. At the time of a containment failure, simulation of the mass-transport controlled release of radionuclides and their outward migration through the waste package begins. The AREST code contains modules that describe the thermal, geochemical, and hydrological environments of simulated waste package. These modules, in turn, depend upon the output from engineering/research codes external to AREST. The reliance upon external support codes gives AREST great power and flexibility. Computing times are not excessive and new models can easily be incorporated without major programming changes. More importantly, with the aid of information supplied by appropriate site-specific support code calculations, AREST can be used to assess the performance of a wide range of geologic media, repository configurations, and waste package designs.

INTRODUCTION

The Office of Geologic Repositories (OGR) of the U. S. Department of Energy (DOE) is currently developing a strategy for assessing the performance of radioactive wastes stored permanently in a deep geologic repository. Because of the time scales involved, (thousands of years and greater) the OGR performance assessment strategy must necessarily rely upon computerized models of the geologic repository system and its components.

The EBS is one component of the geologic repository system. The AREST code, which is being developed by Pacific Northwest Laboratories (PNL) for the OGR, is designed to provide a quantitative assessment of the performance of both individual barrier materials and the overall EBS relative to regulatory requirements for the containment and isolation of nuclear wastes. As such, it can serve as the source-term component of a code (or codes) designed to evaluate the overall performance of the entire geologic repository system.

Essentially, the AREST code is an executive code designed to simulate the containment-and-release performance of individual waste packages under a wide range of environmental conditions, repository and waste package design configurations, and receipt scenarios. The main features of the AREST code are its stochastic framework, its use of mechanistic models of chemical and physical processes, the manner in which these process models have been integrated into the overall stochastic structure, and its reliance upon support codes. The AREST code incorporates the output from detailed research codes in such a manner that computational efficiency is gained without the corresponding decrease in accuracy that often results from the use of simplified models and approximations. The purpose of this paper is to describe the current status of the AREST code.

OVERVIEW OF THE AREST CODE

Conceptually, the AREST model consists of three major components, each of which pertains to some stage of the containment-release process. These submodels, which have been described elsewhere in the literature, (1-3) are the:

- Engineered System Release (ESR) model
- Waste Package Containment (WPC) model
- Waste Package Release (WPR) model.

The AREST code is designed to simulate individual waste packages. The WPC code simulates those corrosion processes and degradation mechanisms that ultimately result in the failure of the waste package container (and optionally, other metallic barriers such as Zircaloy cladding) to isolate the waste form. The containment phase of the simulation is completed at the time physical containment is lost and the possibility for release of radionuclides from the waste package exists. When the waste package containment phase ends, the WPR code begins to simulate the mass-transport controlled release of radionuclides and their migration outward through the waste package. Finally, the ESR code integrates (sums) the simulated radionuclide releases from individual waste packages with respect to their failure-time distribution to provide an estimate of the total repository release. The ESR code also controls the flow of information among the various components and submodels of the AREST code.

Waste package containment and release cannot be simulated without information about the environment in which these processes occur. The AREST code contains modules that utilize detailed information about the thermal, geochemical, and hydrological environments in which the waste package and the repository exist. The thermal module provides the thermal information required by other components of AREST; temperatures are updated at each time step of each simulation. The geochemical module provides the values of the variables used to describe groundwater composition in the vicinity of the waste package. The values of groundwater variables are also updated at each time step. The hydrologic module is used to determine the time that elapses, following emplacement and subsequent repository closure, until resaturation occurs at the waste package surface. Models are currently being developed that describe the mechanical stresses to which the metallic barriers are subjected and the effects of the radiation to which they are exposed.

A common feature of the waste package environmental modules is their use of information provided by support codes that are external to AREST. These external support codes are engineering/research codes that perform calculations that are too time-consuming to do within a simulation code. Output from the support codes is tabulated or otherwise preprocessed for input to AREST. This feature provides great power and flexibility because it enables AREST, which is a performance assessment code, to take advantage of the accuracy and state-of-the-art capability available in detailed research codes without sacrificing required computational efficiency. Moreover, AREST does not depend on any particular support code, so new modeling developments can be incorporated simply by changing support codes without the need to make major programming changes in the code. Finally, AREST can be used to assess performance for a wide range of repository sites and/or geologic media with the information supplied by appropriate site-specific support code calculations.

Figure 1 shows the major components of AREST. Their relationships to 1) the support codes, 2) the models that describe the waste package environment, and 3) the required input modules and input variables are also shown. Detailed descriptions of these components are presented in subsequent sections.

WASTE PACKAGE ENVIRONMENT

At its present stage of development, the AREST code contains modules that describe the thermal, geochemical and hydrological environments of the simulated waste package. A mechanical stress module is being developed and the inclusion of a radiation-effects module is being considered.

Thermal Model

In AREST, temperatures for simulated waste packages are calculated with the aid of the temperature-time profile of a preselected reference case or design-basis waste package. The calculation of waste package temperature proceeds as follows. First, an initial temperature is simulated. The temperature of the simulated waste package at subsequent times is computed using the assumption that, at all times, the elevation in temperature of the simulated container above the ambient repository temperature is proportional to the elevation in temperature of the reference-case waste package. The temperature of the simulated waste package can be expressed mathematically as follows:

$$\frac{T_s(t) - T_a(t)}{T_r(t) - T_a(t)} = \frac{T_s(0) - T_a(0)}{T_r(0) - T_a(0)}$$

or, equivalently,

$$T_s(t) = \frac{T_s(0) - T_a(0)}{T_r(0) - T_a(0)} [T_r(t) - T_a(t)] + T_a(t)$$

where

$T_s(t)$ = temperature of the simulated waste package container at time t,

$T_r(t)$ = temperature of the reference case waste package at time t,

$T_a(t)$ = ambient repository temperature at time t.

When t=0, $T_s(0)$, $T_r(0)$, and $T_a(0)$ refer respectively to the initial temperatures of the simulated waste package, the reference waste package, and the repository.

The initial waste package temperatures, $T_s(0)$, are obtained by sampling from a distribution of initial waste package temperatures. The distribution of initial waste package temperatures is derived, in turn, from a distribution of initial waste package heat generation rates. The conversion of heat generation rates to initial waste package temperatures is site-specific and depends on the thermal properties of the host medium.

The distribution of heat generation rates depends upon assumed spent-fuel characteristics and repository receipt scenarios. The analysis is currently performed using WASTES II as a support code, and is based on the receipt scenario described in the 1985 DOE Mission Plan for the Civilian Radioactive Waste Management Program (4,5). The PNL spent fuel data base provides reactor-specific discharge information (based on the 1984 Energy Information Administration middle case nuclear growth projection) to WASTES II, which in turn maintains the age and exposure of each discharged batch of assemblies and calculates the heat generation of the spent fuel received at the repository (6). The reference fuel for thermal calculations is ten-year old pressurized water reactor (PWR) spent fuel with an exposure of 33,000 MWD/MTU. Although the current emplacement schedule extends over a period of 25 years, simultaneous emplacement of waste package containers is assumed for modeling purposes.

The reference-case waste package temperature histories are obtained with waste package and repository-scale models using the ANSYS finite element code (7). This code is a widely used, general-purpose finite-element code with both structural and thermal capabilities. Three-dimensional scale models are used to estimate short-term (<1000 years) waste package temperatures. One-dimensional scale models are used to

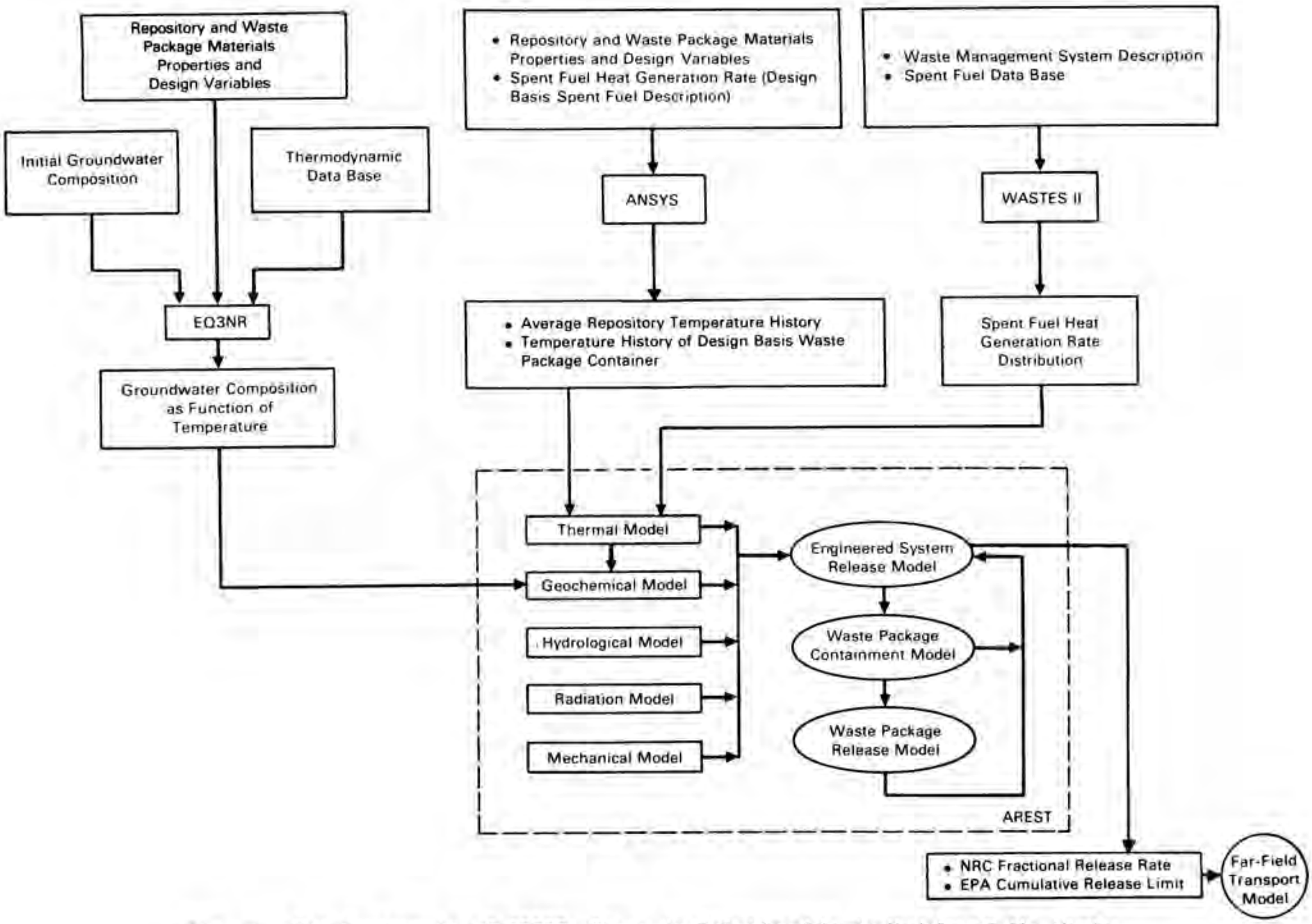

Fig. 1. The Components of AREST, Shown in Relationship to Models of the Waste Package Environment and Required Support Code.

estimate the repository average temperature. The repository average temperatures are combined with container temperatures to estimate long-term (>1000 years) temperatures (8). Temperature histories are tabulated for input to the AREST code.

By means of support codes such as ANSYS and WASTES II, AREST can be used to model the effects on release of various receipt scenarios and the emplacement of different waste types. The analysis can be readily modified to deal with the storage of vitrified wastes.

Geochemical Model

The geochemical model provides information to the AREST code concerning the composition of groundwater within the repository. The composition of groundwater is affected by mass transfer reactions between the groundwater and solids in the host rock, packing material, container, and waste form. These reactions are controlled by factors that include temperature, initial goundwater composition, the solubility of solid phases in contact with the groundwater, and the distribution of the aqueous mass among the various chemical species in solution.

The equilibrium speciation/solubility code EQ3NR is used to generate groundwater compositions that are tabulated for use by the AREST code (9). With the aid of the groundwater compositions reported in the environmental assessment reports for the potential repository sites, EQ3NR is used to compute the aqueous equilibria for specific host rock and waste package designs (10-12). In the case of a bedded salt repository, limitations introduced by the lack of thermodynamic data relevant to high ionic-strength brines at elevated temperatures precludes the use of the EQ3NR code to predict compositions. For those cases, compositions were estimated from experimental data.

Hydrological Model

The National Academy of Sciences has cited evidence to support the assumption that diffusive transport is the expected mechanism for nuclide migration within waste packages at each of the three candidate sites (13). This assumption is further supported by information in the environmental assessment reports produced for the candidate repository sites (10-12). Accordingly, it is assumed for AREST that the transport of both stable and radioactive species from the waste package is anticipated to be diffusion-controlled at all sites.

Radionuclide release calculations rely on the existence of interconnected pathways of water-filled pores in barrier materials. Thus, the degree of saturation (i.e., a field measure of the percent volume of voids or pores that are filled with groundwater), is an approximate correction factor for mass transfer calculations. The degree of saturation is supplied by the hydrological model for various barrier material and host rock combinations.

Related to the degree of saturation is the time of resaturation (the time to achieve resaturation at the waste package following its emplacement and subsequent repository closure). Resaturation is a complex phenomenon that may involve thermal conduction, groundwater boiling, fracture sealing, and other processes. Consequently, the AREST code relies on simplified bounding calculations to determine the time of resaturation. For ductile, plastic rocks such as salt, it is assumed that resaturation is instantaneous (<10 years) relative to the time scale of interest for nuclear waste containment and release assessment. For unsaturated rock media such as tuff, the time of resaturation is determined by calculating the time at which the waste package environment cools below the boiling point of water. For competent saturated host rock such as basalt or granite, it is assumed that resaturation time by fluid flow into the unsaturated voids is inversely proportional to rock mass permeability (14).

WASTE PACKAGE CONTAINMENT

Current strategies for demonstrating compliance with Nuclear Regulatory Commission (NRC) "substantially complete containment" performance objective rely upon metallic containers as the primary engineered barrier (10-12, 15, 16). Because corrosion processes are the main failure mechanisms to which metallic containers will be subjected, AREST is currently configured to model various forms of corrosion, including uniform corrosion, pitting corrosion, and stress corrosion. These corrosion models can be applied to the waste package container and, optionally, to other metallic barriers such as Zircaloy cladding. Moreover, the code can accommodate situations in which containment by a specified percentage of the waste packages has been lost at or prior to the time of emplacement.

For uniform corrosion, the basic requirement of the AREST code is a module that can calculate the rate of corrosion as a function of relevant environmental variables, such as temperature and pH. A linear approximation of this corrosion rate is used to determine the loss in container thickness at each time step of a waste package simulation. Several mechanistic models of the rate of uniform corrosion, as well as empirical models derived from site-specific testing, have been preprogrammed for inclusion in AREST. The pitting corrosion model combines a rate function with a probabilistic model that describes the number and location of pits. Because the rate of pit growth is a function of depth, the pitting corrosion module is linked to the uniform corrosion module. A simple mechanistic model of stress corrosion is currently available.

"Corrosion" is a term that describes a wide variety of complex material-specific phenomena that involve chemical or electrochemical interactions between the material and the environment. A comprehensive corrosion model is not deemed possible because not all the mechanisms associated with corrosion are well understood and may not be desirable in multiple waste package simulations because of the complexity of the processes involved. Furthermore, the environments into which the barrier materials will be placed has not yet been fully characterized. For these reasons, the simulation of waste package performance by AREST is no more reliable than currently-available, site-specific corrosion models and supporting data. Consequently, AREST has been designed so that one of several rate functions (modules) for both uniform and pitting corrosion can be selected by the user for each performance assessment. As is the case with external support models, AREST is not identified with or constrained by the use of any particular corrosion model. It is intended that currently-available mechanistic and empirical corrosion models in AREST will be revised or replaced as newer, more reliable models appear. The strategy of using mechanistic corrosion models in AREST whenever possible has been adopted because there is some question concerning the acceptability of empirical models for performance assessment (16). Figure 2 shows the WPC model in relationship to other components of AREST.

Uniform Corrosion

A uniform corrosion model, originally developed by Chao et al. to describe the growth of continuous passive films, has been adapted for use in AREST (17). In order to relate the model of Chao et al. to the rate of uniform corrosion, it is assumed that the rate of corrosion of the material in question is the same as the rate of film buildup on its surface. The validity of this assumption is unresolved and currently under investigation. It is further noted that the time spans involved in modeling container corrosion are considerably longer than those of interest for the development of thin corrosion films.

Several additional models of the rate of uniform corrosion have been programmed as AREST modules. These include the Basalt Waste Isolation Project (BWIP) model of uniform corrosion, a model of uniform corrosion in a salt environment, and a model developed for the Nuclear Regulatory Commission (18-20). All three models are empirical and all predict the rate of uniform corrosion of a steel container. The BWIP model, like the mechanistic model of Chao et al., takes different forms in aqueous and steam environments.

Pitting Corrosion

Pitting corrosion is a local phenomenon that can cause rapid penetration of a metallic specimen. Once a pit is initiated, a local electrochemical environment quite different than that of the bulk solution is produced and maintained, so that pit growth can be quite rapid. Because the initiation and growth of pits in a ferrous material is a highly variable stochastic phenomenon, a probabilistic model of pitting corrosion been incorporated into the AREST code. The probabilistic model requires a module that can calculate the rate of pit growth at each time step. Although the probabilistic aspects of the pitting model are an integral part of the AREST code, the pit growth rate model is coded as an external module that can easily be modified or replaced.

For modeling purposes, the number of potential pit sites in a waste package container is assumed to follow a Poisson distribution. In addition, the pit sites are assumed to be randomly located over the surface of the waste package container. The assumption that all pitting sites are at the container surface is conservative in the sense that it leads to earlier failures than would be the case if the pit sites are assumed to be distributed throughout the container. At each time step in the simulation of a waste package, the rates of uniform corrosion and pitting corrosion are compared to

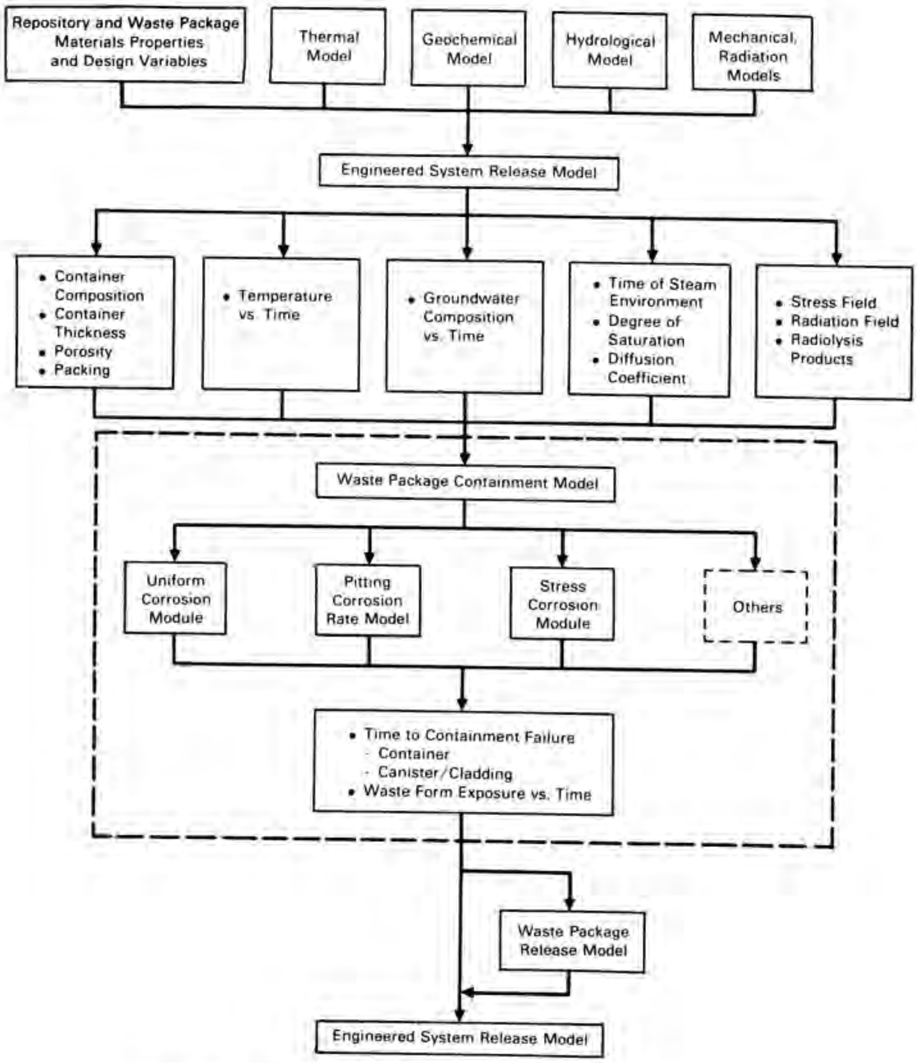

Fig. 2. The Waste Package Containment Model

determine if pitting begins at additional pit sites. Upon initiation of pitting at a potential site, the increase in pit depth is computed at each subsequent time step. The simulation of pitting corrosion ceases when it is determined that the number of pits that have penetrated the container exceeds a specified percentage of the area of the inner wall of the container. For this calculation, it is assumed that all pits have constant cross-sectional area that does not change with depth. The percentage of the container inner wall surface area that constitutes failure is an input variable.

One model selected to describe the pitting growth rate is that of Stahl and Miller (21). The model treats pitting as a one-dimensional transport process that is limited by diffusion of the metal cation through a dilute binary electrolyte. Diffusion is driven, in turn, by concentration and potential gradients. Other pitting growth rate models have been proposed (see Reference 20, for example), but most use an enhancement factor that is applied to the rate of uniform corrosion. Such growth rate models are unsatisfactory because a comparison of the rates of uniform corrosion and pitting corrosion to determine if pitting is initiated results in a conclusion that either pitting begins at all potential sites or that it begins at no potential sites. The development and use of any pitting model are hampered by the lack of an adequate data base.

Stress Corrosion

A simple mechanistic model for predicting the rate of stress corrosion cracking of the waste package container is currently available for use with AREST. The stress corrosion module in AREST is based on the work of Newman and uses the stress intensity supplied by the mechanical module to predict crack tip velocity at a point of stress cracking at each time step (22). Because stress relaxation occurs with time and the current mechanical module does not take this into account, the model is conservative in that it predicts more rapid penetrations (earlier failures) in a given situation than would realistically be expected.

The present stress corrosion rate model has been developed for highly caustic environments, so there is some question about its applicability to the candidate repository sites. Moreover, stress corrosion is a highly variable phenomenon, and the WPC module does not presently incorporate this variability.

WASTE PACKAGE RELEASE

The NRC has established quantitative performance objectives for the allowable fractional release rate of radionuclides from an EBS (15, 16). The NRC has defined the EBS, but there are alternate interpretations of the definition of the EBS boundary. To avoid confusion and to preserve technical conservatism, the AREST code assesses releases from the waste package subsystem of the EBS. Although releases from the EBS can be no greater than from the waste package, EBS releases may be significantly lower than releases from the waste package.

The WPR model of the AREST code also calculates cumulative releases of radionuclides from the waste package of the EBS for the 10,000 year period following repository closure. The cumulative releases are used to evaluate waste package performance relative to limits set by the Environmental Protection Agency (EPA) (23). Although the EPA limits on cumulative release are imposed at the accessible environment boundary (several kilometers from the waste package), comparison of the waste package subsystem with overall repository system requirements is judged to provide an additional, useful perspective for safety assessment purposes.

Figure 3 shows the general structure of the WPR model for spent fuel. The model requires the failure time of each simulated waste package container as input. (Alternately, realizations from an arbitrary user-defined probability distribution can be used, but in that case ties with the values of variables that affect failure time may be severed.) Release calculations are based upon two mass transfer models, one for solubility-limited release and one for inventory-limited release (24, 25). The advantages and the application of mass transfer theory to calculate releases are discussed elsewhere in the technical literature (24-27).

Solubility-Limited Release

The AREST code implements equations that have been derived with the aid of mass transfer theory to describe the time-dependent diffusive mass transport of radionuclides away from a waste package (24). Specifically, a mass transfer rate is calculated as a function of time and location within the waste package. The mass transfer equations are based on a model of waste package geometry that consists of three nested regions: an inner region that is assumed to be an impermeable spherical waste form equal in area to the (inner) surface area of the actual cylindrical waste form container; a porous region surrounding the waste form, either a tailored packing material or equivalent barrier, and a porous host rock extending infinitely in all directions. Calculations for a prolate spheroid geometry (chosen to closely approximate the actual cylindrical geometry of a waste package), have been compared with those for the spherical geometry. It was found that waste package releases for the two geometries were nearly equal when the surface areas were made equal (24).

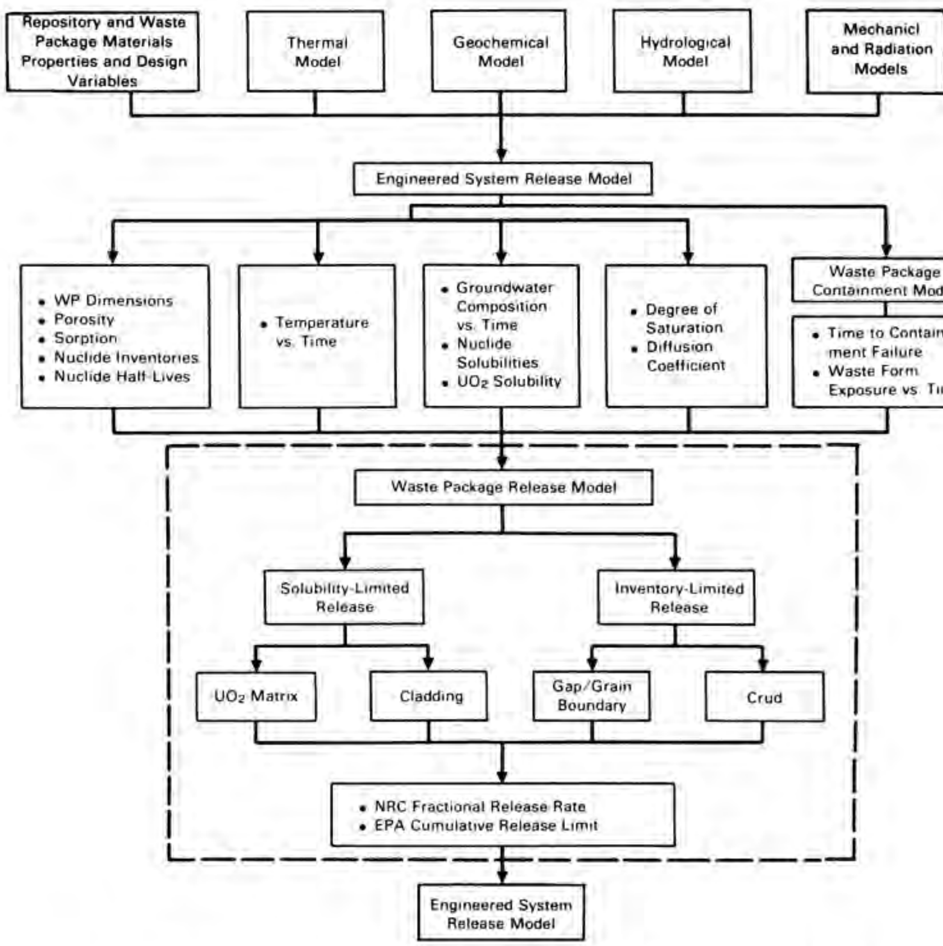

Fig. 3. The Waste Package Release Model as Implemeted for Spent Fuel.

The mass transfer rate calculated for this "solubility-limited" model is a function of the following variables:

- the nuclide concentrations at the waste form surface
- the radioactive decay constants
- the aqueous-phase diffusion coefficient
- the radial dimensions of the waste form and thickness of packing
- the nuclide retardation coefficients for packing and host rock
- the porosities of packing and host rock.

In addition, the release rates can be scaled to account for the degree of hydrologic saturation and the limited exposure of the spent fuel surface area (26).

An initial boundary condition is imposed that fixes the concentration of each radionuclide at the waste form surface. These fixed values can be solubility-limited concentrations imposed by a discrete radionuclide-bearing solid (24). In general, the surface concentrations for different nuclides cannot be assumed equal or otherwise related to each other, so the mass transfer rates will differ from one radionuclide to another (i.e., the case of incongruent release).

Alternately, congruent dissolution of the waste form may occur, so that instantaneous fractional release rates at the waste form surface are equal for all components. In that case, the release rate for each radionuclide is directly proportional to the solubility of the waste form matrix and the ratio of the masses of the radionuclide and the matrix component.

Inventory-Limited Release

The AREST code implements mass transfer equations that have been derived to describe highly soluble nuclides that will not be solubility-limited but may be assumed to be inventory-limited as released from a waste package (25). These equations are based on a planar geometry that includes a waste form, a saturated void volume adjacent to the waste form, a porous layer of packing (or equivalent material), and the host rock. Dimensions of the barriers in this model are transformed from the actual cylindrical geometry of the waste package. The volume of the void is set equal to the difference in volumes of the cylindrical waste form container and the total volume of the enclosed spent-fuel rods. The surface area is that of the cylindrical waste form container, and is identical to that used in the solubility-limited case.

In relation to the time scale of interest, it is assumed that the void volume fills with water instantaneously at the time of containment failure. A certain mass of the radionuclide is assumed to dissolve from the waste form at the same instant, so that an initial (non-zero) concentration of the radionuclide is achieved. The initial concentration of a soluble radionuclide is computed by dividing its mass by the volume of the water-filled void. Subsequent transport is assumed to be diffusion-controlled.

The inventory-limited mass transfer calculations depend on the following variables:

- the initial concentrations of radionuclides in water-filled void space
- the radioactive decay constants
- the volume and outer surface area of the void space
- the packing thickness
- the aqueous-phase diffusion coefficient
- the radionuclide retardation coefficients for the packing and host rock
- the porosities of the packing and host rock.

The inventory-limited release model incorporates decreasing mass flux from both radioactive decay of the source and depletion because of diffusion out of the region of fixed initial inventory.

Limitations of Mass Transfer Analysis

The use of currently available mass transfer models to calculate releases involves certain limitations. First, the models cannot account for the effect of spatial inhomogenieties on release. The present models assume a set of concentric spheres, each shell of which has uniform properties. However, unpublished results by the Basalt Waste Isolation Project indicate that releases from a cylindrical waste package capped by a region with significantly different porosity than the host rock may be preferentially channeled through this cap. Second, current mass transfer models in the WPR model do not explicitly consider colloid transport. This limitation stems more from the lack of suitable data (e.g., size spectrum, sorption/filtration effects, agglomeration rates) than from the limitation of mass transfer models themselves.

Diffusion through groundwater, without the effect of tortuosity, is the assumed limiting transport mechanism. Surface diffusion along clay mineral surface has been proposed as a faster pathway of release for some radionuclides. If this or similar mechanisms for preferential transport can be confirmed under realistic repository conditions, then the effective-diffusion coefficients in the mass transfer equations can be revised to handle this situation.

The effect of adjoining waste packages is not currently considered in the WPR model. The assumption that releases from individual waste packages are unaffected by releases from neighboring waste packages is believed to be conservative because elevated radionuclide concentrations in the host rock from waste packages that fail early can only decrease the rates of release from subsequent waste packages.

The use of reversible sorption coefficients (K_d), which assume equilibrium conditions to calculate retardation coefficients of radionuclides, expedites the incorporation of many separate chemical interations, but this approach has not been shown to be conservative. However, with the exception of short-lived radionuclides, reversible sorption within the waste package subsystem does not sensitively affect the calculation of significantly steady-state release rates because of the short distance between the waste form and the boundary of the waste package. Steady-state release rates at long time are independent of reversible sorption. Current models do not incorporate irreversible sorption (ion exchange), although this process could greatly attenuate waste package releases (28).

Finally, the mass transfer equations used in the WPR model are simplified. More complex mass transfer models lead to more realistic, and usually, *more* favorable estimates of expected performance. Given the current availability of information and uncertainties in the data, the simplified and defensibly conservative models being used to expedite iterative calculations are judged to be appropriate.

ENGINEERED SYSTEM (INTEGRATED) RELEASE

The ESR model serves two purposes. First, it combines the calculations of the WPC and WPR models to provide a time-integrated estimate of total repository release. Second, it monitors and controls the flow of information among all the components of AREST and its various process modules and support codes.

The one purpose of the ESR model is to combine the releases calculated for individual waste packages to provide a time-integrated estimate of total repository release (the source-term). The method for calculating the source-term is essentially the same as that used by Sagar et al. and is also used in a report prepared for the NRC by the Aerospace Corporation (29, 30). The source-term is calculated from the individual waste package releases by means of the following formula:

$$\sum_i R_i(t,\tau_i) = \sum_i R(t,\tau_i)$$

$$= \sum_i R(t - \tau_i) = \sum_i \int_0^{t-\tau_i} r(t')dt'$$

where $\{\tau_i\}$ is a series of waste package failure times, $R_i(t,\tau_i)$ is the total release up to time t from a waste package that fails at time τ_i, and $r(\tau')$ is the time-dependent release rate for an individual waste package.

It is currently assumed that $R_i(t,\tau_i) = R(t,\tau_i)$, or equivalently, that all waste packages have the same release function. It is further assumed that $R(t,\tau_i) = R(t-\tau_i)$, or that release depends only on the elapsed time since failure. This latter assumptions implies that the shape of the release function does not change with the time of waste package failure. Computationally, these assumptions mean that the release function need be calculated only once for all waste packages, rather than individually for each waste package.

As noted earlier, the effect of adjoining waste packages is not currently considered in the calculation of releases from individual waste packages. Likewise, this effect is not considered in the calculation of integrated releases; integrated releases are calculated under the implicit assumption that each waste package behaves independently of all others.

A second purpose of the ESR model is to monitor and control the flow of information among the components of AREST. To the extent possible, these tasks have been localized in the ESR module, both to preserve modularity and to minimize the code that must be modified when additional feedback loops are introduced among the components of AREST. A key aspect of information control is to ensure that updated information is passed from the waste package environment modules to the WPC and WPR modules at each time step. In particular, these modules require updated temperatures and groundwater compositions. The ESR module controls inputs to ensure that they have the necessary information to perform updated calculations.

The WPC module performs the containment phase of a waste package simulation, and the WPR module begins the simulation of release at the time containment failure is indicated. The time of failure, together with the temperature and the values of there environmental variables at the time of failure, are passed from the WPC module to the WPR module by the ESR module. The containment and release phases of a waste package simulation are clearly interdependent and should therefore be performed jointly. However, it is possible with the aid of the ESR module to use either of the WPC or WPR modules separately. The ESR module can be used to generate a series of waste package failure times from an arbitrary distribution. These times are used by the WPR module to perform release calculations that are independent of specific corrosion mechanisms and waste package designs. On the other hand, the WPC module can be used to estimate the containment performance of various waste package designs under the specific input conditions without the need to perform subsequent release calculations. This feature contributes greatly to the flexibility of the AREST code.

SUMMARY

The AREST code is being developed to aid in the assessment of the EBS of a geologic repository system. The conceptual model that guides the code development has been described in the technical literature (1-3). The philosophy used in developing AREST has been to integrate mechanistic models of corrosion and release into a unified probabilistic framework. The code, which has been designed for flexibility and computation efficiency, relies upon a number of research/scientific codes to provide detailed information about the repository environment. In particular, support codes provide detailed information about the temperature and groundwater composition in the waste package environment. The code is capable of simulating corrosion processes that affect metallic barriers, including uniform corrosion, pitting corrosion, and stress corrosion. Available corrosion modules employ both mechanistic and empirical models. Models of radionuclide release based on mass transfer theory are used to calculate release rates. Models have been developed for the cases in which release is solubility limited and inventory limited, and they are applicable to engineered systems with multiple barriers. To date, the release models have been implemented only for spent fuel, but they can also be used to evaluate the performance of other waste forms. The code has been used to assess the adequacy of spent fuel as a waste form (31).

Because the AREST code is currently in a stage of active development, this paper serves to document progress to date. Plans for future work include the following: 1) develop improved ways to model spatial variability, 2) use more detailed and comprehensive models for thermal calculations, 3) improve the numerical efficiency of release calculations and extend their application to other waste forms, 4) introduce models of disruptive geologic events, and 5) addition of modified release models for the precipitation of radionuclid-bearing phases within the waste package. Verification and benchmarking activities are also being conducted.

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