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REVIEW OF WAPPA - A WASTE PACKAGE SYSTEM PERFORMANCE CODE

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ABSTRACT

The potential of WAPPA, a second-generation waste package system code, to meet the needs of the regulatory community are analyzed. The analysis is based on the contents of the code manual, a letter-form update of the code and, to a lesser extent, on the source program. The analysis is structured in two main sections encompassing an in-depth review of WAPPA's individual process models and a review of WAPPA's operation, respectively. The analysis lists and discusses potential problems in the use of WAPPA. It is concluded that the code is of limited use to the NRC in the present form. Recommendations for future improvement, usage, and implementation of the code are also given.

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Introduction

Of three individual-barriers performance criteria in 10 CFR 60 two are directly concerned with waste package behavior after repository closure. The criteria require that the waste package should contain the waste for a period of 300 to 1,000 years, and that following the containment period, the engineered barrier system, i.e., the waste package and the underground facility, should limit the annual release of any radionuclide to no more than one part in 10^5 of that radionuclide's inventory at 1,000 years.

So far, two codes have been developed for integrated, waste package performance analysis: BARIER and WAPPA. Of the two, WAPPA is DOE's preferred code. Further development of BARIER has been discontinued and WAPPA is presently used by the Salt and Tuff repository programs. The Basalt program does not have a code such as WAPPA or BARIER.

The objective of this report is to examine WAPPA's level of modeling to determine its potential uses for the regulatory community.

Review of WAPPA's Process Models

The Waste Package Performance Assessment Code WAPPA was constructed for general applicability to all candidate geologic media, to any waste type, and to conventional waste package designs and geometries. The code was designed to serve as a tool in all of the following major areas: waste package design, repository design, site selection and characterization, and system assessment.

WAPPA consists of about 13,000 source program statements representing five physical process models and a system drive model for integrated waste package performance assessment. With reference to Figure ES.1, the five process models include radiation modeling, thermal modeling, mechanical modeling, corrosion modeling, and leach-and-transport modeling. These models are

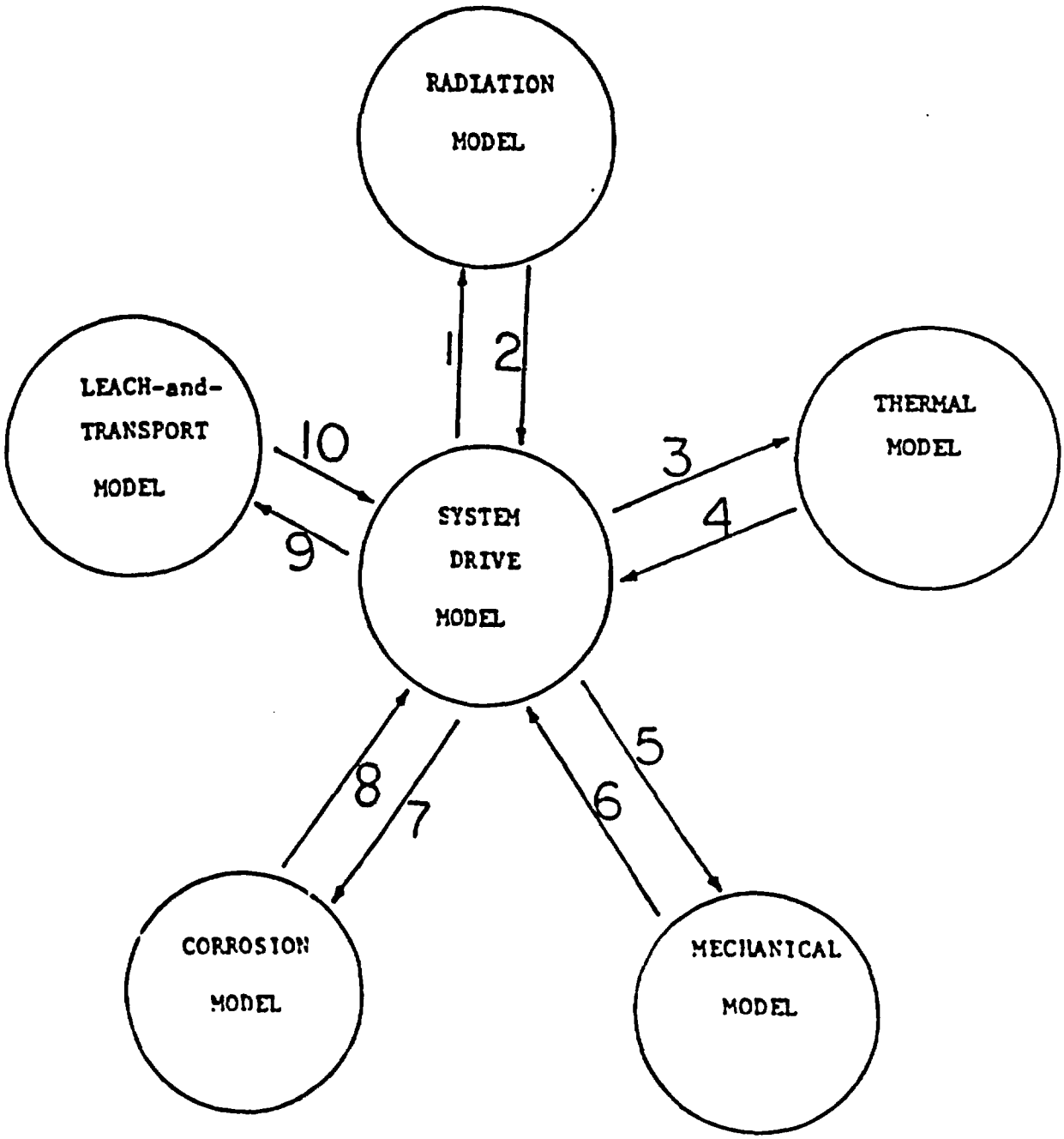

Figure ES-1 Schematic Representation of how WAPPA operates within each time step.

sequentially activated in the above order within each time step by the system drive model. Each process model applies to all waste package barriers at the same time. For instance the radiation model would determine the radiation field throughout the waste package as well as corrosion and leaching enhancement factors for wetted barriers. Thus, the implemented approach is termed "barrier-integrated and process-sequential." The code uses one-dimensional, radial axisymmetric geometry with correction factors for finite height effects.

Radiation Model

The Radiation Model calculates decay heat, radionuclide, gamma, and alpha source terms and empirical factors to account for radiation enhanced leaching, corrosion, and waste form degradation. The decay heat, gamma and alpha dose rates, and radionuclide mass inventory are obtained by interpolation, as a function of time, from a user supplied table. Total doses are obtained using a simple first order integration of the dose rates. The alpha particle dose is used to obtain an empirical estimate of the degradation of thermal conductivity, fracture strength, thermal expansion coefficient, and density of the waste form. Empirical leaching and corrosion enhancement factors accounting for radiolysis effects are obtained by interpolation, as a function of gamma dose and flux, from user supplied tables.

Thermal Model

The Thermal Model uses the decay power from the Radiation Model and a user supplied time-dependent temperature at the waste package boundary to calculate the steady-state temperature profile within the waste package from analytical expressions. Three modes of heat transfer are considered: conductive, convective, and radiative. Convective heat transfer is modeled through the use of an equivalent conductivity. Radiative heat transport is allowed only in gas gaps. When radiative heat transport is present, the resulting equations are non-linear with respect to temperature and an iterative solution procedure is used. The temperatures computed in the Thermal Model are used in the three remaining process models.

Mechanical Model

The Mechanical Model calculates the stresses in the waste form and barriers in order to assess stress-assisted fracture. The Mechanical Model contains three coupled submodels: (a) the Stress Analysis Submodel which calculates the stress on each barrier; (b) the Canister Fracture Submodel which determines if the metal barriers fracture; and (c) the Waste Form Fracture Submodel which determines if the waste form fractures and thereby increases the surface area available for leaching.

Corrosion Model

The Corrosion Model calculates the type and amount of chemical degradation of metallic barriers and determines when the relevant process causes these barriers to fail. The Corrosion Model considers general corrosion; localized corrosion, including pitting and crevice corrosion; stress corrosion, including stress corrosion cracking and hydrogen embrittlement; galvanic corrosion; and dry oxidation. These processes are treated through empirical correlations supplied by the user in the form of tables of corrosion rates as a function of relevant parameters such as temperature or stress. If a barrier fails during a time step, it is conservatively assumed that the failure occurred instantaneously at the beginning of the time step and the groundwater contacts the next barrier immediately.

Leach-and-Transport Model

The Leach-and-Transport Model is executed following failure of the barrier next to the waste form. This model calculates the release rate of nuclides from the waste form, their transport out of the repository, and the accumulated mass of each nuclide delivered to the repository. The leach rate submodel includes both dissolution and diffusion from the waste form and is modified by empirical correlations to account for the effects of temperature, radiation, solution saturation, and waste form fracturing. The transport submodel through breached metal barriers uses a steady-state diffusion equation.

If packing materials are present, they are considered to be saturated with groundwater. Transport through this region is computed using a transient mixing cell model which accounts for diffusion, advection, and retardation through adsorption.

Conclusions

The main shortcoming of WAPPA's implemented modeling approach is that the process models are not self-standing, i.e., they imply a large number of assumptions and rely heavily on empirical correlations and user-provided inputs. For practical applications and acceptability of the results, it will behoove the user to make sure that all assumptions that went into the modeling are indeed warranted for the problem at hand, and that the data used are indeed relevant. Both tasks are significant and may prove to be overwhelming as they may require comparison with more detailed analyses and initial information that is difficult to obtain from or it may not even exist in the literature.

Review of WAPPA's Operation

WAPPA's modeling approach is more empirical than mechanistic, which places the user in the position of preparing extensive input and support data files to run the code for each problem at hand.

Input Specifications

Input specifications to the code include geometrical configuration and materials of the waste package; calculation times; nuclides to be tracked during the calculations; temperature, fluid flux, vertical stress, and radial stress at the waste package-host rock interface as function of time; packing materials resaturation time; radiation decay properties, radiation shielding properties, empirical data for radiation damage, thermal properties, mechanical properties, empirical data for end effects on stress analysis, empirical data for corrosion, and empirical data for leaching; radionuclide, gamma and

alpha inventories as function of time; and thermal power as function of time. Some of these data have to be supplied as function of several variables such as temperature, pH, etc.

Output Specifications

WAPPA allows many options to control the amount of data to be printed. Options exist for echo prints of the input as well as the output of results generated during execution.

Conclusions

The input to WAPPA can only be prepared by qualified personnel who are thoroughly acquainted with the assumptions that went into the formulation of each process model.

Difficulties in preparing the input and support data files will arise for two main reasons. First, some of the input data require a pre-knowledge of how the waste package would perform. Second, the data may be difficult to obtain or it may not even exist in the literature. Furthermore, because of the magnitude of the task, any WAPPA user will probably be limited to use data which factor in only a few of the system variables on which they depend. Thus it will also be necessary for the code user to show that the reference data are conservative.

WAPPA's implemented numerical strategy lacks internal control of the time step and of numerical errors. This may lead to unnecessary conservatism and places on the user the extra burden of redefining the time step vector and re-running the code several times in order to make sure that convergence is achieved.

Conclusions and Recommendations

WAPPA is a modular code to determine system performance of high level nuclear waste packages in groundwater saturated porous media. The code logic is conservative and the modeling level is simple, as expected in a system code.

WAPPA implements a modeling approach that is mostly empirical in nature. In practice, it operates as a data base manager that simply selects which correlation and which data are applicable to each particular situation. Because of the large amount of data the user has to supply for the empirical models and the number of situations for which they may have to be specified, data gathering, interpretation, and validation will require a significant effort by personnel who are thoroughly familiar with the assumptions that went into the code. The difficulty of preparing the data files will be compounded by the scarce availability of adequate data in the literature and by ambiguities the required data may entail, e.g., data are needed which require a priori estimate of future waste package performance; and data are needed for correlations which factor in only a few of the several variables on which a particular process may depend. Furthermore, since most of the models are empirical, their applicability must be proven. This will require a suite of auxiliary codes representing state-of-the-art modeling of the actual processes considered.

While usage of WAPPA as a licensing tool requires extensive data and model validation, one may relax these requirements for code usage as a site screening tool or as a tool for preliminary design analysis. It will be necessary, however, to remove first some of the major inconsistencies identified in the modeling, e.g., the leach-and-transport model needs to be modified to conserve mass, etc. WAPPA is hardly amenable to probabilistic reliability analysis because of the large number of parameters to be sampled and the need to re-run the code a number of times to insure convergence. The last difficulty may be hard to remove even if sensitivity analysis is performed first.

In its present form, the WAPPA code is of limited use to the NRC. However, because of WAPPA's importance within the DOE programs, the NRC should maintain a code running capability and future updates of the code for ready reference.

If DOE indicates that relevant licensing information will be provided through WAPPA, it is suggested that the NRC request the DOE to prepare an in-depth data preparation manual.

1. INTRODUCTION

1.1 BACKGROUND INFORMATION

The Code of Federal Regulations in its Part 10 CFR 60 §60.113 (June 1983) requires that the applicant for a license to operate a nuclear waste repository demonstrate compliance of the proposed design with the following performance criteria of individual barriers after permanent closure:

1. Containment of HLW within the waste packages should be substantially complete for a period to be determined by the Nuclear Regulatory Commission. Such a period shall be no less than 300 years and no more than 1,000 years.

2. The release rate of any radionuclide from the engineered barrier system following the containment period should not exceed one part in 100,000 per year of the inventory of that radionuclide calculated to be present at 1,000 years. Exception to this rule is allowed for radionuclides whose release rate is less than 0.1% of the calculated total release rate limit, which is taken to be 1 part in 100,000 per year of the (total) inventory of radioactive waste that remains after 1,000 years of radioactive decay.

3. Pre-waste-emplacement groundwater travel time along the fastest path of likely radionuclide travel from the disturbed zone to the accessible environment should be at least 1,000 years or such other travel time as may be approved or specified by the Nuclear Regulatory Commission.

Although the controlled release requirement is on the engineered barrier system (the waste package and the underground facility), it is expected that the applicant will rely primarily on the waste package portion of the system. Thus, waste package performance is the direct concern of 2 out of 3 NRC individual-barrier performance criteria.

So far two waste-package system performance codes have been developed: BARIER and WAPPA, in chronological order. Both codes were developed for the Salt Program,[1,2] but were kept general enough to be applied to hard rock repositories. At present, development of the code BARIER has been discontinued, and WAPPA is the only code of the Salt and Tuff Programs for integrated waste package performance. In particular, the Tuff Program is modifying WAPPA to allow its use for nonsaturated conditions. The Basalt Program does not have a waste-package system code.

This document presents a review of the code WAPPA as it is presented in the code manual ONWI-452 of April 1983 and in a subsequent, letter-form update of December 1983 by the code custodian.[3] For clarity, the code WAPPA is briefly introduced in Section 1.2. This document's objectives and organization are presented in Section 1.3.

1.2 THE CODE WAPPA

The Waste Package Performance Assessment Code WAPPA was constructed for general applicability to all candidate geologic media, to any waste type, and to conventional waste package designs and geometries. The code was designed to serve as a tool in all of the following major areas: waste package design, repository design, site selection and characterization, and system assessment.

WAPPA consists of about 13,000 source program statements representing five physical process models and a system drive model. With reference to Figure 1.0, the five process models include radiation modeling, thermal modeling, mechanical modeling, corrosion modeling, and leach-and-transport modeling. These models are sequentially activated in the above order within each time step by the system drive model. Each process model applies to all waste package barriers at the same time. For instance the radiation model would determine the radiation field throughout the waste package as well as corrosion and leaching enhancement factors for wetted barriers. Thus, the implemented appr ach is termed "barrier-integrated and process-sequential."

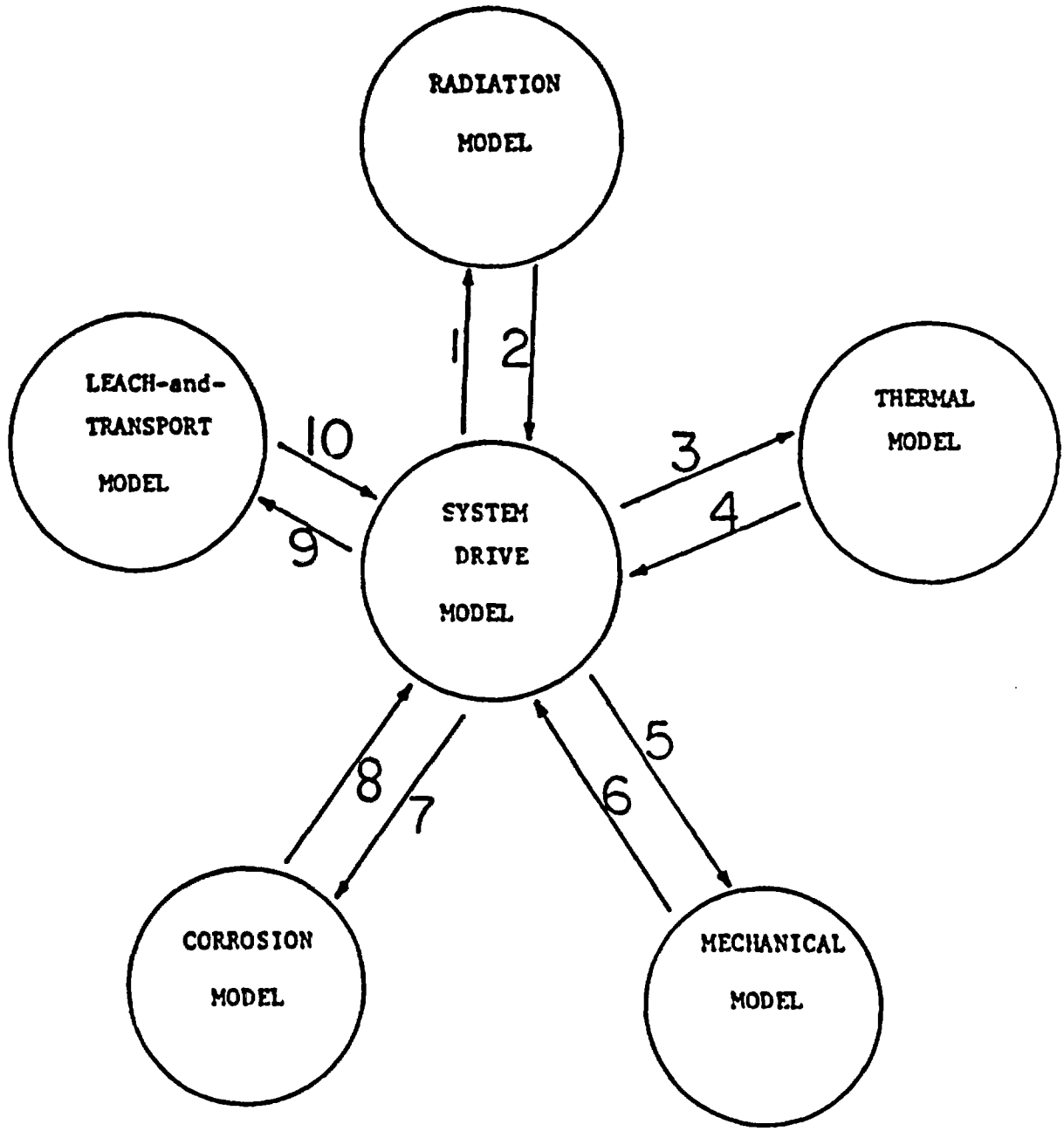

Figure 1.0 Schematic Representation of how WAPPA operates within each time step.

The code uses one-dimensional, radial axisymmetric geometry with correction factors for finite height effects.

The modeling approach implemented in WAPPA is more empirical than mechanistic. Thus a most significant but little emphasized task in the operation of WAPPA is the preparation of a data base encompassing all empirical parameters for the problem at hand. The task can be overwhelming due to the recognized lack of pertinent data in the literature and to the large variation of problems one may have to solve.

1.3 OBJECTIVES AND ORGANIZATION OF THIS REPORT

The present review of WAPPA has been prompted by the importance of this code within the DOE community which regards it as the preferred code for integrated waste package analysis.

The objective of this report is to examine the code's level of modeling in order to determine its potential uses for the regulatory community, i.e., whether the code could be used for licensing, reliability analysis, screening of various waste package designs, etc. Furthermore, we have also examined the possibility of adapting parts of WAPPA into existing codes at BNL.

Chronologically, we have first run the code at BNL and examined the Complex Verification Test Case provided by the code developer. This indicated some potential problems in the code modeling and its structure. We then examined each process model following the code manual and, to some extent, the source program. This effort also resulted in re-writing part of the Leach-and-Transport model. Our findings were documented in a series of memos-to-file which were made available to the NRC and its contractors.[4-12]

The present report draws on the material of our original memoranda. With minor changes they constitute Chapters 2 and 3 of the document, and deal with each process model and WAPPA's operation, respectively. Conclusions are drawn in Chapter 4, which also gives our final recommendations.

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2. REVIEW OF WAPPA'S PROCESS MODELS

As indicated earlier, the code WAPPA was constructed for general applicability to all candidate geologic media, to any waste type, and to conventional waste package designs.

The code uses one-dimensional, radial axisymmetric geometry with correction factors for finite height effects, where applicable. System performance is determined through sequential usage of five main process models representing radiation modeling, thermal modeling, mechanical modeling, corrosion modeling, and leach-and-transport modeling. With reference to Figure 1.0, sequential coupling in the above order is operated by a system drive model. Thus, within each time step, results from the Radiation Model can be used in the four remaining process models, results from the Thermal Model can be used in the three remaining models, and so on.

Presented hereafter is a review of all five process models. Each model is reviewed separately in Sections 2.1 through 2.5. General conclusions about WAPPA's level of modeling are drawn in Section 2.6.

2.1 WAPPA'S RADIATION MODEL (RMODEL)

The primary function of the radiation model is to calculate radiation induced effects that are required as input to other WAPPA process models. Thus, the radiation model obtains the decay heat rate which is used by the thermal model, the alpha damage to the waste form to be used in the mechanical model, and corrosion and leaching enhancement factors due to radiolysis to be used in the corrosion and leach-and-transport models, respectively. These effects are simulated through four distinct submodels which are titled as follows: (a) Source Term, (b) Attenuation, (c) Radiolysis, and (d) Damage. A description of each submodel is presented next. A discussion follows in Section 2.1.2. Conclusions are drawn in Section 2.1.3.

2.1.1 Review of Modeling Approach

2.1.1.1 Source Term Submodel

The first function of this submodel is to obtain the decay heat rate, gamma ray and alpha particle emission rate, and radionuclide mass inventory within the waste form at any given time. The basis of the calculation is a logarithmic interpolation procedure using a user supplied time-dependent data base. Presently, this data base is prepared by using the isotope buildup and decay code ORIGEN2.

The second function of this submodel is to calculate the gamma dose and the alpha particle displacement dose at the waste form periphery. The alpha particle displacement dose is used by the Damage submodel to calculate degradation of waste form properties. The gamma dose is used by the Radiolysis submodel to calculate enhancement of corrosion and leaching caused by gamma radiolysis. It should be emphasized that this gamma dose is at the periphery of the waste form and not in the groundwater where the radiolysis occurs.

2.1.1.2 Attenuation Submodel

This submodel calculates the attenuation of gamma rays as they travel from the waste form to the repository. This is accomplished by calculating the gamma flux as a product of the source in the waste form, a buildup factor, and an attenuation factor. The empirical buildup factor simulates the effect of scattered radiation. The attenuation factor is a function of the thickness and type of barriers in the waste package.

2.1.1.3 Radiolysis Submodel

WAPPA assumes that the influence of gamma radiolysis on corrosion and leaching can be modeled through empirically determined enhancement factors. These are multiplicative factors defined so that multiplication of the leach or corrosion rate by the enhancement factor gives the enhanced rate due to

radiolysis. The radiolysis submodel determines these enhancement factors, as function of the gamma flux, dose rate and cumulative dose at the edge of the waste form, through a logarithmic interpolation of user supplied data.

2.1.1.4 Damage Submodel

This submodel calculates changes in the thermal conductivity, fracture strength, thermal expansion coefficient and density of the waste form due to alpha-induced damage. These properties remain unchanged until the alpha displacement dose reaches a user defined critical value. After reaching this value, the material property under consideration is degraded according to a saturating exponential which depends on the cumulative dose and empirically determined coefficients.

2.1.2 Discussion

WAPPA's radiation submodels primary method of calculating a desired quantity involves reading a data base. This causes two problems. First, the input required for the data base may not be readily available. If this is the situation, the required information could be obtained through ad hoc experiments or through use of more advanced computer simulations. For example, assuming that the buildup factor in basalt is unknown, a detailed photon transport calculation could be performed and the buildup factor chosen such that the flux as calculated by the transport code matched the flux calculated by WAPPA's attenuation submodel. The second problem is that each user must construct his own data base. WAPPA does not supply the data. It does not even supply a list of references where the appropriate data can be found. This makes tne calculation subject to the user's ability to obtain the proper data. Because of the paucity of present data, and the uncertainty in some of them, it is unlikely that any two users will create the same data base. Additional comments regarding each particular submodel are offered as follows.

2.1.2.1 Source Term Submodel

The Source Term submodel's major function involves reading waste-form inventory information from a data base. The modeling it implements does have two conservative approximations: (1) it does not account for redistribution of nuclides due to leaching; therefore it overpredicts the radiation source within the waste form; and (2) it uses the gamma flux and total dose at the waste form periphery for determining enhancement of leaching and corrosion, which overpredicts the effects of radiolysis. Indeed, during the containment period the flux at the waste form periphery will be much greater than in the groundwater. Thus, the calculated total dose to the groundwater will exceed the actual dose. Since the enhancement is a function of both dose and flux, radiolysis effects are overpredicted. The magnitude of the overprediction will be larger for leaching enhancement as compared to corrosion enhancement because leaching appears to be more sensitive to radiolysis.

2.1.2.2 Attenuation Submodel

The attenuation submodel serves no obvious purpose. Currently, the only use for the gamma flux is to determine the amount of radiolysis that occurs in the groundwater. However, since WAPPA uses the gamma flux at the waste form boundary, as determined in the Source Term submodel, calculations of the flux in the remainder of the waste package are superfluous.

Assuming that future revisions of the code do use the gamma flux within the waste package, the following comments become relevant.

The documentation for this submodel lacks detail and justifies this shortcoming on the claim that the model uses standard expressions from the Reactor Shielding Design Manual.[1] However, it turns out that the equations are applied incorrectly in WAPPA. The error involves improper definition of the buildup factors. Before explaining this error, a description of buildup factors and their properties is presented.

Buildup Factors

WAPPA assumes the effects of scattered radiation can be accounted for through a buildup factor. This prevents the need for a detailed transport calculation. However, it requires the use of an empirically determined build-up factor, defined as the ratio of the total flux to the uncollided flux. As the distance travelled by the gamma rays increases, the proportion of scattered flux to the total flux increases. Therefore, the buildup factor increases with distance. This does not imply the total flux increases with distance, in fact it decreases with distance as the total flux is the product of a buildup factor and an attenuation factor which decreases faster than the buildup factor increases.

Error in the Buildup Factor

Viewing Figure 2.0, and noting that WAPPA approximates the gamma radiation from the cylindrical waste form as originating from an infinite line source, the error made in WAPPA can be explained. For a gamma ray originating within the line segment $d\ell$, it must travel a distance R to reach point P. However, WAPPA calculates the buildup factor based on the normal distance between the line source and point P, the distance a+z in Figure 2.0. Because $(a+z) < R$ and the buildup factors increase with distance, this assumption is non-conservative. Heuristic arguments,[2] indicate the calculated flux will be within a factor of 10 of the flux obtained using the distance R in calculating the buildup factor. Considering the uncertainties in the entire calculation and the fact that corrosion or leaching will be enhanced by less than 20 percent for an order of magnitude increase in gamma dose, this error may not be significant, but it should be addressed in the code manual.

Empirical Coefficients in Buildup Factor Expression

Furthermore, although WAPPA claims to use standard formulae, the expression for the buildup factor uses slightly different definitions for the

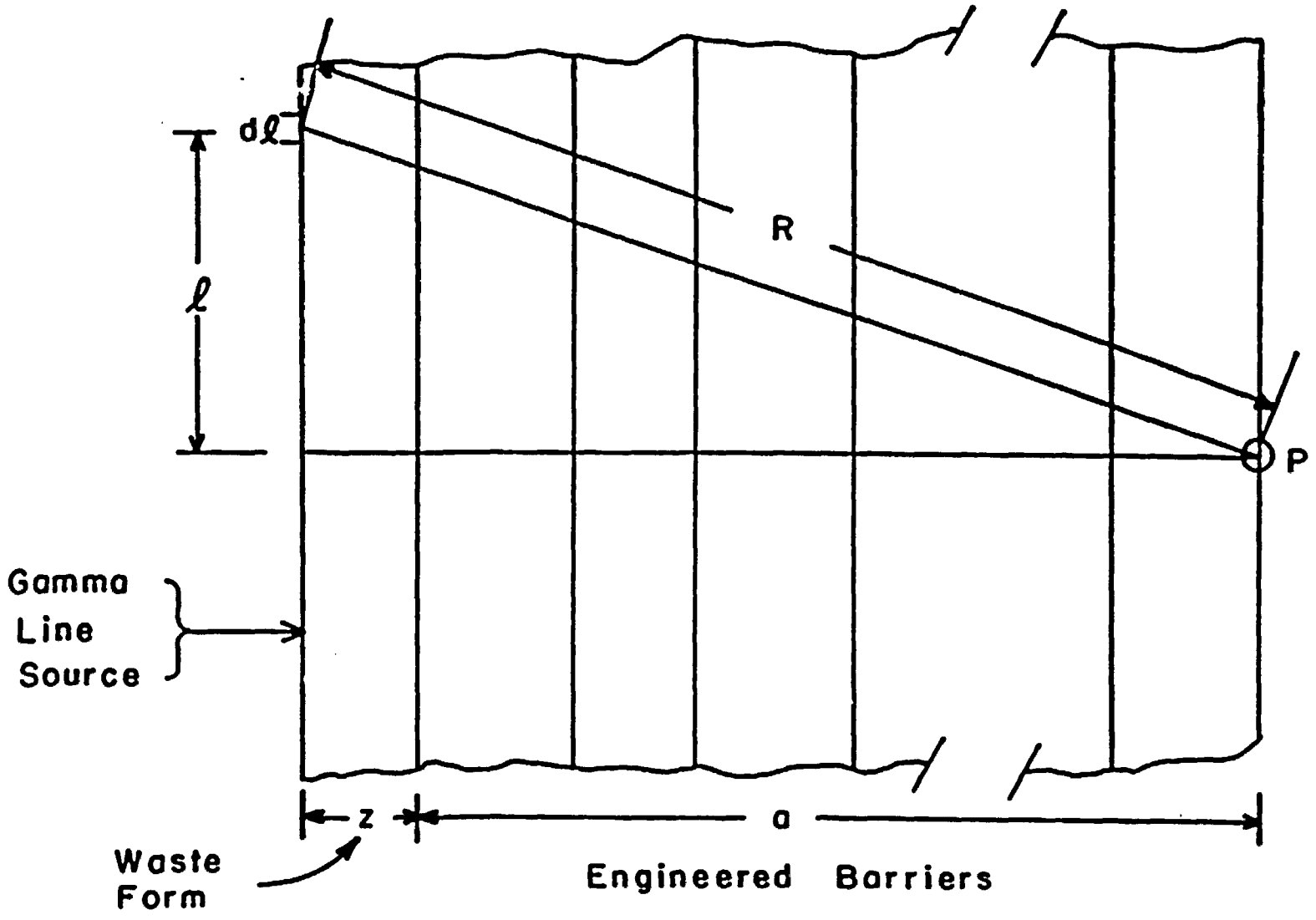


Figure 2.0 Geometrical representation of the waste form as a line source surrounded by the engineered barriers of the wate package.

empirical coefficients when compared to the definitions found in the Reactor Shielding Design Manual,[1] the reference for buildup factors cited by WAPPA.

WAPPA defines the buildup factor B_i for material "i" as:

$$B_i = A_{1i}e^{-\alpha_{1i}t_i} + A_{2i}e^{-\alpha_{2i}t_i} \qquad (2.1)$$

where A_{1i}, A_{2i}, α_{1i}, and α_{2i} are material dependent empirical coefficients and t_i is the thickness of material "i" normal to the line source. In contrast, the Reactor Shielding Design Manual defines the buildup factor as:

$$B_i = A_{1i}e^{-k_{1i}\mu_i T_i} + A_{2i}e^{-k_{2i}\mu_i T_i} \qquad (2.2)$$

where A_{1i}, A_{2i}, k_{1i}, and k_{2i} are material dependent empirical coefficients and μ_i is the adsorption coefficient of the medium, and T_i is the thickness of medium that the gamma ray passes through.

From these two expressions it is clear that

$$a_{ji} = k_{ji}\mu_i \qquad j = 1,2 \qquad (2.3)$$

and the equations are similar. However, this discrepancy is not pointed out in the manual.

2.1.2.3 Radiolysis Submodel

The Radiolysis submodel has the following limitations.

WAPPA calculates only one leach enchancement factor. This assumes that radiolysis has the same effect on all waste form constituents. However, radiolysis changes the number and types of ionic species present in the groundwater. This in turn influences the solubilities of the different species in the groundwater and alters the leach rates from the waste form. Each species will react differently to these radiation induced changes.

WAPPA does not model alpha radiolysis nor does it attempt to account for the gamma flux in the groundwater that arises from particles leached from the waste form. Once leaching begins, alpha and gamma emitting species enter the groundwater. Alpha particles do not interact with the groundwater in the same manner as gamma rays.[3] Therefore, the water chemistry is different and leaching from the waste form will respond accordingly. This effect may be negligible because the amount of alpha and gamma emitting nuclides in the groundwater should be small.

The WAPPA manual does not mention the possibility of colloid formation due to gamma irradiation in salt repositories.[4] In principle, this could be handled through leach and corrosion enhancement factors as currently done in WAPPA.

Lack of a detailed water chemistry model in WAPPA limits any attempt at modeling radiolysis effects to be heuristic and prone to be at most qualitatively correct. The accuracy of the radiolysis model is totally dependent on external justification.

2.1.2.4 Damage Submodel

The Damage submodel has the following limitations.

Although the idea that alpha damage can be represented as a saturating exponential function of the total dose is not new, the data base to support this is limited. This may be a particular problem for glass. The reference cited in WAPPA[5] that proposes the saturating exponential correlation bases its model on experimental results on radiation effects in crystalline ceramic materials. The other radiation damage reference[6] does consider glass, however the data reported is for one glass composition and does not provide data for all of the radiation-induced property changes used in WAPPA.

The damage submodel does not attempt to calculate a leach enhancement factor due to alpha damage of the waste form. Apparently this was considered at one time by the developers of WAPPA because the empirical coefficients for

the saturating exponential correlation are requested as input. However, these coefficients are unused. The manual does not justify neglecting this effect.

2.1.3 Conclusions

All of the submodels used to evaluate radiation-induced phenomena are structured to rely heavily on a user supplied data base. Assuming the data are available, the radiation model might provide a conservative estimate of the processes it models. Use of a data base approach allows the models to be simple and the computational times short. However, it also places a large burden on the user. Furthermore, because of the large quantity of data requested, coupled with the uncertainty in some data, it is unlikely any two users will develop the same data base.

2.2 WAPPA'S THERMAL MODEL (TMODEL)

WAPPA's Thermal Model computes the temperature profile within the waste package and feeds it to the System Drive Model for updating temperature dependent parameters in the Mechanical, Corrosion, and Leach-and-Transport models. Following a description of the modeling approach in Section 2.2.1, Section 2.2.2 discusses the limitations of the implemented submodels. Conclusions are drawn in Section 2.2.3.

2.2.1 Review of Modeling Approach

WAPPA's thermal modeling approach rests on the assumption that the heat capacity of waste package barriers is negligible and that the temperature distribution is a function only of radial distance from the waste form centerline. In the waste form it is assumed that the heat source is uniform. Solution of the resulting steady-state heat conduction equation yields then a parabolic temperature distribution.[7] In the cylindrical annulus representing the various waste package barriers it is assumed that there is no generation of heat. Solution of the heat conduction equation in this region without a source results then in a logarithmic profile.[7] In terms of the

temperatures at the waste form centerline and at the interfaces between adjoining barriers, the waste package temperature profile is expressed as follows:

$$T_o = T_1 + \frac{q'(t) r_1^2}{4\, k_0(T_1)} \tag{2.4}$$

$$T_i = T_{i+1} + \frac{Q_i(t)}{2\pi H\, k_i(T_{i+1})} \ln (r_{i+1}/r_i), \quad i=1,2,\ldots,N \tag{2.5}$$

where T_o is the centerline temperature; T_1 is the temperature at the waste form periphery; r_i is the distance of the i-th interface from the waste form centerline; $T_i = T(r_i,t)$; $q'(t)$ is the volumetric heat generation rate in the waste form; H is the height of the waste package; $k_0(T_1)$ is the effective thermal conductivity of the waste form; $k_i(T_{i+1})$ is the effective thermal conductivity of the i-th barrier based on the temperature at the outer edge of the barrier; $Q_i(t)$ is the effective, total conductive heat flux out of the i-th interface.

Heat transfer by convection is considered important in liquid or gas filled annuli when the Grashof number exceeds 20,000. The Grashof number is a dimensionless parameter defined as:

$$N_{GR} = \frac{X^3\, \rho^2\, g\, \beta_f\, \Delta T}{\mu^2} \tag{2.6}$$

where X is the gap width; ρ is the density of the fluid; g is the acceleration due to gravity; β_f is the volumetric expansion coefficient; ΔT is the temperature difference across the gap; and μ is the fluid viscosity. When convection is important, the parameter k_i in Equation (2.5) is the familiar thermal conductivity corrected through an equivalent conduction enhancement factor which is a function of the Grashof number.

Heat transfer by radiation is considered for gas filled annuli and is modeled through modification of the conductive heat flux. Thus, for gas gaps, the quantity $Q_i(t)$ used in Equation (2.5) is the total heat flux minus the total radiative heat flux, $q_i(t)$, which is defined as follows:

$$q_i = A_i F_{i,i+1} \sigma (T_i^4 - T_{i+1}^4), \tag{2.9}$$

where:

A_i - area of i-th interface

$F_{i,i+1}$ - view factor from i-th to (i+1)-th interface

σ - Stefan-Boltzmann constant.

Radiation heat transport will be most important during the first few years after burial when the heat source and temperature gradients through the waste package are largest.

Equations (2.4) and (2.5) can be solved sequentially once either the temperature at the waste form centerline or the temperature at the waste package-host rock interface is specified as function of time. The Thermal Model adopts the second one as the reference temperature. The waste package-host rock interface temperature is provided in the code as a user supplied table of temperature data versus time.

The above formulation is abandoned when the total heat generation rate becomes less than 1 watt. At that time, a few hundred years, all temperatures within the waste package are set equal to the user-provided, reference repository temperature.

2.2.2 Discussion

WAPPA's assumed parabolic-logarithmic temperature profile within the waste package is the profile that would exist in the system if this had had infinite time to equilibrate thermally with its surroundings while the heat

generation rates were kept constant. As such, it would certainly yield a conservative estimate of waste package temperatures if, at any time t, the user-supplied boundary temperature were the thermally equilibrated value. Engineering judgement, however, suggests that, after the first few months during which heat storage effects in the waste package are important, Equations (2.4) and (2.5) closely represent the shape of the waste package temperature profile. Therefore, the accuracy of WAPPA's temperature estimates within the waste package after the first few months rests on the accuracy of the user supplied boundary temperature data. If these data are in error by X degrees, the calculated temperature profile is displaced by the same number of degrees in the waste package.

Since the waste package-repository boundary temperature depends on waste package dimensions and heat generation rates as well as on repository properties, such as rock thermal properties, waste package arrangement, area thermal load, etc., the present Thermal Model logic would call for a large data base of boundary temperature values versus time. In analogous situations, other researchers have preferred to couple the waste package thermal model, Equations (2.4) and (2.5), with a thermal code for the repository. Both options would require substantial improvement of WAPPA.

WAPPA is inadequate for reliable temperature prediction during the first few months after burial as the Thermal Model formulation breaks down in the limit when heat storage effects in the the waste package are important. However, the model would still provide reasonable estimates of internal waste package temperatures provided an "appropriate" set of boundary temperature data is supplied by the user.

2.2.3 Conclusions

WAPPA's thermal model usefulness for short-term temperature prediction, i.e., during the first few months after burial, is limited to providing conservative estimates of waste package temperatures by selecting "appropriate"

values for the user-supplied boundary temperature. Reliable, short-term temperature prediction would require adding a temperature submodel to the code which include heat storage effects.

WAPPA's thermal model may provide reliable estimates of waste package temperatures a few months after burial provided the user-supplied data base of boundary temperatures is shown to be accurate. This may require a separate run of a repository thermal code which takes into account waste package heat generation rates and dimensions as well as waste package arrangement, rock thermal properties, etc.

2.3 WAPPA'S MECHANICAL MODEL (FMODEL)

In WAPPA's modeling approach three types of stress-assisted breaching of waste package barriers can occur: 1. stress corrosion cracking of metallic barriers, 2. fracture of metallic barriers at pre-existing cracks, and 3. brittle fracture of the waste form.

The purpose of FMODEL is to predict the magnitude of local stresses (stress intensity factors) at pre-existing flaws on metal surfaces, and to determine the extent to which the waste form fractures due to the applied stress. These tasks are accomplished by coupling a Canister Fracture (CF) Submodel and a Waste Form fracture (WF) Submodel to a Stress Analysis (SA) Submodel. These submodels are introduced next. A discussion follows in Section 2.3.2. Conclusions are drawn in Section 2.3.3.

2.3.1 Review of Modeling Approach

2.3.1.1 Canister Fracture Submodel

Given the calculated stress level by the SA submodel and the user-specified length of pre-existing cracks on metallic barriers, the CF submodel computes empirical, elastic stress intensity factors.

If the metal has not yielded plastically, the stress intensity factor is compared with the metal's critical value of fracture toughness. Breaching occurs when the stress intensity factor exceeds the fracture toughness.

If the metal has already yielded plastically, a new effective crack length is calculated. The stress intensity factor is then recomputed and compared with the fracture toughness of the material.

The equations used in this submodel are empirical in nature. Therefore one must make sure they apply to the materials, loading pattern, and configurational geometry at hand. To that effect, the CF submodel write-up does not give useful references, therefore these equations must be accepted with reservations.

2.3.1.2 Waste Form Fracture Submodel

Given the various components of the stress as calculated by the SA submodel, the WF submodel checks for regions where tensile stresses exceed the fracture strength of the material. Since the problem is regarded as axisymmetric, this defines an outer annulus where the waste form is fractured. The volume of the fractured region is then multiplied by an empirical coefficient to determine an equivalent surface-area increase later to be used by the Leach-and-Transport Model.

2.3.1.3 Stress Analysis Submodel

While the CF and WF submodels are empirical in nature, the SA submodel is based on the classical theories of strength of materials and stress analysis.

From a strength analysis point of view, the FMODEL considers five types of materials whose properties are modeled as follows:

1. The waste form is modeled as an elastic/brittle material which undergoes fracture in the region where tensile stresses exceed the waste form fracture strength.

2. Metallic barriers are modeled as elastic/plastic materials. These materials yield plastically in regions where the TRESCA criterion is satisfied. Namely, when

$$\text{Max}\left(|\sigma_r-\sigma_\theta|,\ |\sigma_\theta-\sigma_z|,\ |\sigma_r-\sigma_z|\right) \geq \sigma_{yield}$$

3. Packing materials are modeled as compressible elastic elements. They yield, i.e., they are extruded, when the Von Mises maximum stress exceeds the yield stress. That is when:

$$\sigma_{max} = \frac{3}{2}\sqrt{(\sigma_r-\sigma_H)^2 + (\sigma_\theta-\sigma_H)^2 + (\sigma_z-\sigma_H)^2} > \sigma_{yield},$$

σ_H being the hydrostatic pressure.

4. Gas gaps are modeled as having zero pressure and no stress transfer capability.

5. Liquid gaps are modeled as incompressible elements. Also, all "failed" portion of barriers, i.e., the fractured waste form region, the plastically yielded portion of metallic barriers, and all corrosion layers are treated as incompressible elements.

From a stress analysis point of view, the modeling approach regards the waste package as a series of concentrical cylindrical annuli encircling a solid core. The length of the waste package is infinite and loading is of the compressive type in both the horizontal and vertical directions. Horizontal loading is due to the repository confining horizontal pressure, to thermal expansion, and to initial residual stresses at the canister/waste form interface. Vertical loading is due to the repository vertical confining pressure. No shear, torsion, or bending is accounted for, nor are gravity loading and friction between components. As a result, all deformations take place horizontally in the radial direction. Stress enhancement due to the finite height of the waste package is handled through an empirical factor which multiplies the calculated stress.

2.3.2 Discussion

2.3.2.1 Limitations of the Implemented Modeling Approach

Any model appearing in a general purpose code like WAPPA can only be expected to handle a few important effects and failure modes. In the case of the FMODEL, the modelers have identified brittle fracture of the waste form and cracking of the metal barriers at pre-existing flaws as the main mechanical failure modes of the waste package. To that end they disregard bending, torsion, gravity loading, friction effects, creep, buckling, etc., which is likely to be an acceptable approach but it is not justified in the document. Also, the expressions used for calculating empirical stress intensity factors at pre-existing cracks are not properly referenced and justified.

The implemented modeling approach does present some desirable features, i.e., it accounts for degradation of mechanical properties due to radiation (empirical factors and data have to be used) and for the influence of temperature on the stress. The model also accounts for initial, residual processing stresses.

The most important limitations are that materials strength, as measured by yield stress and tensile strength, is not modeled to be a function of temperature, and that the volumetric expansion of the corrosion products is not addressed. Corrosion products are known to exert very large pressures in constricted regions, e.g., the phenomenon of denting in nuclear steam generators and the wedging action of corrosion products.[9]

2.3.2.2 Adequacy of the Implemented Modeling Approach

Two relevant waste package failure modes are not given sufficient attention in the implemented modeling approach. These are, 1.) failure of the waste package ends and, 2.) buckling of metal barriers beyond their elastic stability region.

With reference to Figure 2.1, which reports a typical waste package design for high-level waste, it appears that a weak area in the canister structure is the neck area. In that area the metal is not supported by the waste form and the neck shape favors concentration of stresses. Thus, crushing of the air gap appears to be an important failure mode which ought to be addressed. Stresses may also concentrate at the bottom of the canister at the welds between the base and the rest of the metal, thus causing the base to detach. This failure mode should also be addressed.

Furthermore, it should be noted that as the unfailed part of metal barriers becomes progressively thinner due to corrosion and plastic yielding, it may be subject, at one point, to elastic instability, i.e., under sufficiently high stress the cylindrical metal annulus may buckle into an "eight" shape. This is one failure mode in submarines, and may be an important failure mode for waste package performance.

FMODEL uses a number of empirical correlations to represent mechanical behavior of the waste package. For this reason, the ability of FMODEL to provide a conservative estimate of waste form fracture and canister failure can not be guaranteed unless the data used by the correlations can be shown to be conservative.

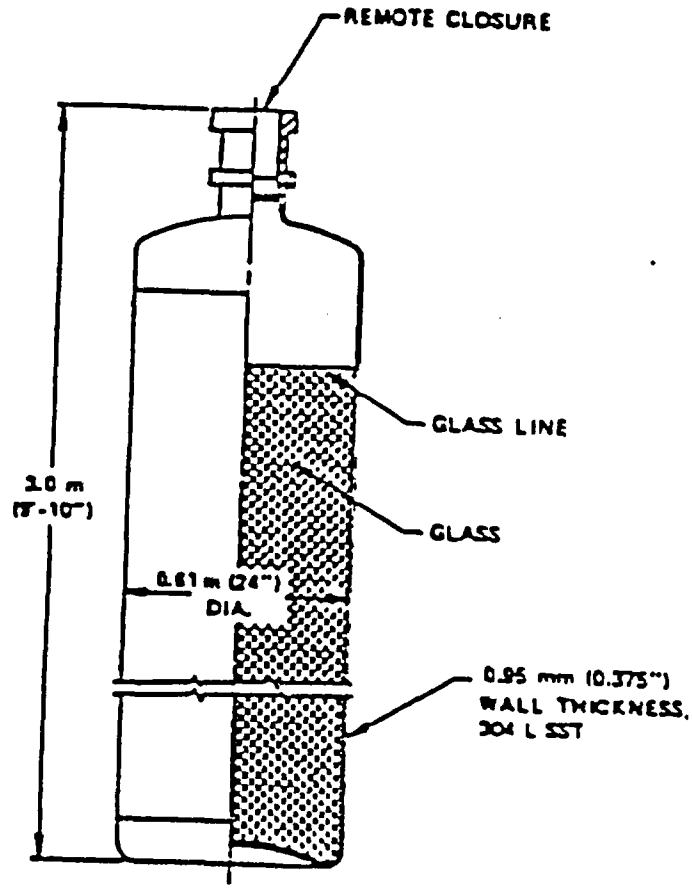


Figure 2.1 Typical waste form and canister design (Adapted from Ref. 8).

2.3.3 Conclusions

The FMODEL cannot be used by itself in a predictive mode. It relies heavily on user-supplied data which may not be obtained from the literature and for which the user may have to make ad hoc experiments. This is the case for important quantities related to failure mode analysis, such as (a) the empirical coefficient to convert waste form fractured volume to an increase in waste surface area, (b) the empirical formulae used to calculate stress intensity factors, and (c) the empirical coefficient to deal with end effects. The FMODEL does not factor in the volumetric expansion of corrosion products which, depending on the degree of fracturing of the host rock, may result in additional confining pressures. Furthermore, the model does not take into account failure of both canister ends nor does it account for the elastic stability of the metal barriers.

2.4 WAPPA'S CORROSION MODEL (CMODEL)

The corrosion model calculates the degradation of each metallic barrier in the waste package due to the following processes:

(1) Dry Oxidation;
(2) General Corrosion;
(3) Galvanic Corrosion;
(4) Localized Corrosion, including pitting and crevice corrosion; and
(5) Stress Corrosion Cracking, including hydrogen embrittlement and active path stress corrosion cracking.

Along with barrier degradation, CMODEL tracks the penetration of water into the waste package as the barriers fail. A description of the corrosion submodels follows next. Section 2.4.2 discusses the limitations of CMODEL. Conclusions are drawn in Section 2.4.3

2.4.1 Review of Modeling Approach

2.4.1.1 Dry Corrosion

Before a barrier is contacted by water, CMODEL considers the spatially uniform one-dimensional thinning of barriers due to oxidation. Oxide growth is calculated by one of three empirical growth laws: logarithmic, parabolic, or a power relation in time. The coefficients required in these laws are defined as a function of temperature through user supplied input tables.

2.4.1.2 Wet Corrosion

Upon wetting of a barrier, wet corrosion models are activated. A distinction is made between mechanisms that cause a uniform degradation of the entire barrier versus mechanisms that cause a local barrier degradation. Uniform corrosion submodels consider galvanic and general corrosion. Local corrosion includes stress corrosion cracking, pitting, and crevice corrosion.

The submodel for galvanic corrosion determines whether water (an electrolyte) is in contact with two adjacent barriers thereby allowing a galvanic cell to form. (This situation can only occur if local corrosion has caused a breach in an outer barrier.) Based on input data, the barrier that acts as the anode is determined and the thickness of this barrier is reduced linearly with time. The rate of degradation is a function of temperature and is increased through the effects of radiolysis. The model does not give credit for cathodic protection.

The model for general corrosion provides a spatially uniform thinning of the barrier. The rate of degradation is determined from an input table, for each barrier, of corrosion rate versus temperature. The effects of radiolysis are incorporated by multiplying the corrosion rate by an enhancement factor which is a function of the gamma dose and flux. The net rate of corroson is a linear function of time.

Local corrosion events are considered "catastrophic". That is, if the conditions required to initiate one of these processes arise, the barrier is considered to breach instantaneously at the beginning of the current time step. Given user supplied empirical data regarding pitting/crevice/crack size and density, the total "breached" area is calculated. Simultaneous with the breach of the barrier, groundwater flows to contact the next barrier.

2.4.2 Discussion

WAPPA's corrosion model was developed with the intention of providing a calculation of the maximum rate of barrier degradation, i.e., a conservative estimate. However, before conservatism can be assured, the following points concerning the data and numerical modeling must be considered.

First, and most important, it is emphasized that all of the corrosion submodels are empirical and extremely data intensive. Corrosion is a complex phenomena that is not understood well from a quantitative, fundamental viewpoint. For this reason, CMODEL uses empirical correlations to supply all the information regarding corrosion rates for each of the various models and for each barrier. The coefficients used in each correlation are supplied by the code user as a function of temperature. No attempt is made at modeling the influence of solution chemistry on corrosion rate. The effect of solution chemistry is assumed to be incorporated into the empirical input supplied by the user. Before CMODEL can be considered conservative, the data used in the empirical correlations must be shown to be conservative over the entire range of potential repository conditions.

Second, the numerical strategy used in CMODEL contains two flaws. The first error involves solution for the amount of dry oxidation, general and/or galvanic corrosion. The solution strategy in WAPPA is process sequential, that is, WAPPA looks at radiation, thermal, mechanical, corrosion, and leaching processes as occurring sequentially in a given time step. In particular, the temperature distribution is calculated before CMODEL calculates the

temperature dependent corrosion rate. If the temperature is decreasing with time, this is the expected condition after the first few hundred years, the corrosion rate is calculated based on a lower temperature and therefore the calculation is non-conservative. This could be corrected through use of the temperature at the previous time step to calculate the amount of corrosion when the temperature is decreasing.

The other error involves solution of the dry oxidation corrosion model. The empirical laws used in calculating oxide thickness are, in general, developed from non-linear, integral-type relationships based on isothermal experimental data. For this non-isothermal system, care must be taken to account for the influence of temperature variations on oxide growth.

The method of solution used in WAPPA for calculating oxide thickness is most easily understood while viewing Figure 2.2, a plot of oxide thickness versus time for two temperatures. For the initial time step, time zero to time t_1, the system is at temperature T_1 and the oxide grows to a depth, d_1. In the subsequent time step, time t_1 to time t_2, the system temperature has been updated and is T_2. WAPPA calculates the incremental oxide growth, Δd_2, as the amount of growth that would have occurred over the time interval t_2-t_1 provided the system had been held at temperature T_2 for the entire calculation time. This growth is represented by the curve through points b and c on the graph. The total oxide thickness is obtained by summation of d_1, the oxide thickness and Δd_2, the incremental growth. Viewing each time step as a new initial value problem, it is seen that the WAPPA code changes the "initial condition" for oxide thickness at each time step. Since growth rate is a function of thickness, this procedure is incorrect.

A better solution procedure is schematically represented in Figure 2.3. Here, after the oxide has grown to a depth d_1 at temperature T_1, time is advanced to the next time step and the temperature is updated and is T_2. In this case, growth of the oxide is calculated starting from a depth d_1 on the isothermal curve for temperature T_2. This is point b in Figure 2.3. Growth progresses along this isothermal curve for a time period corresponding to the

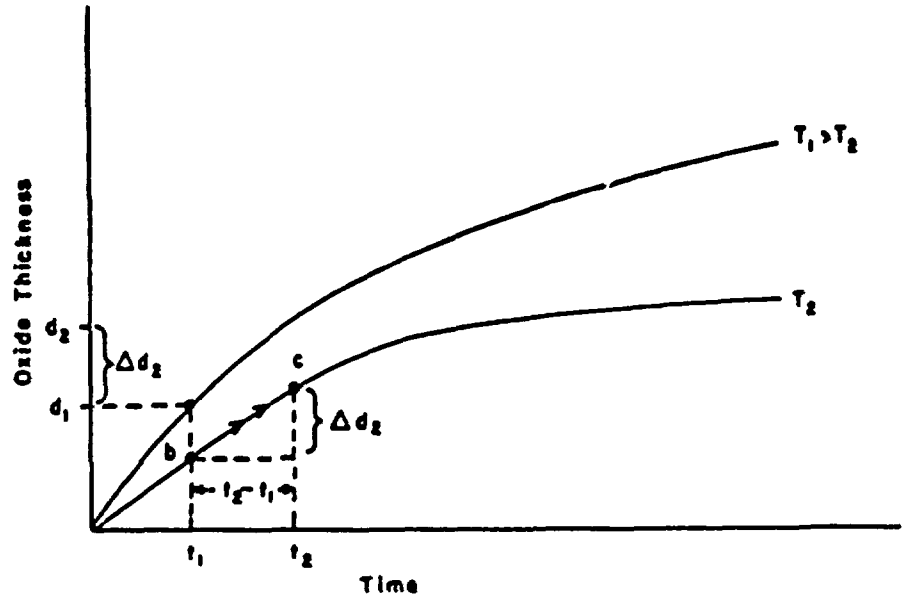


Figure 2.2 Schematic representation of oxide thickness versus time. WAPPA considers thickness as a function of temperature and time.

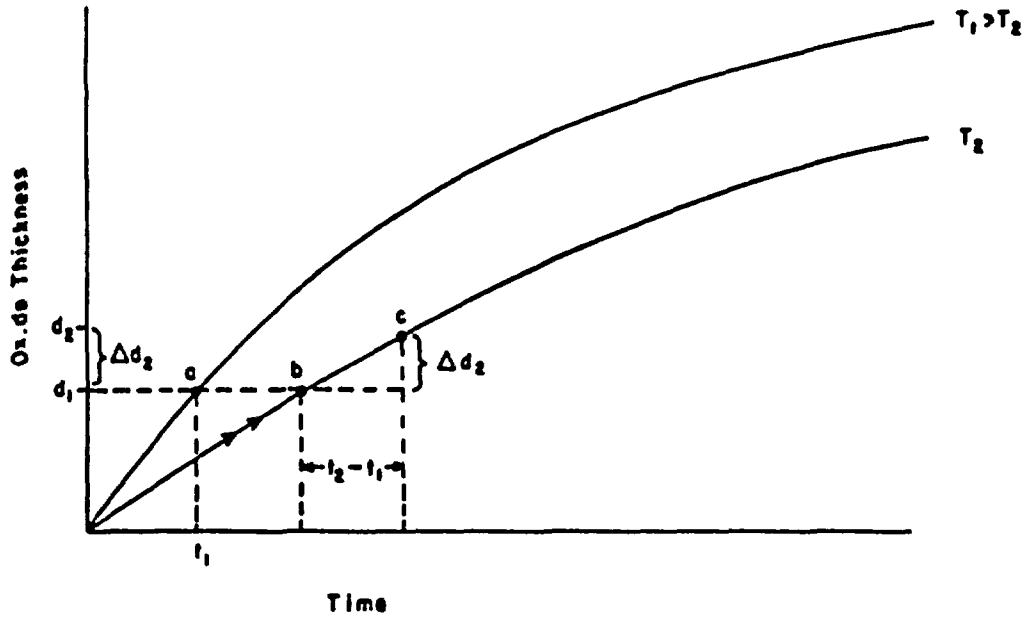


Figure 2.3 Improved oxide thickness calculation considers thickness as a function of temperature and previous history.

length of the time step, $t_2 - t_1$. This is represented by the path between points b and c. The new oxide thickness is the sum of d_1, the initial thickness, and Δd_2, the incremental growth. This model takes the viewpoint that corrosion rate is a function of temperature and oxide thickness whereas the WAPPA model views the corrosion rate as a function of temperature and time.

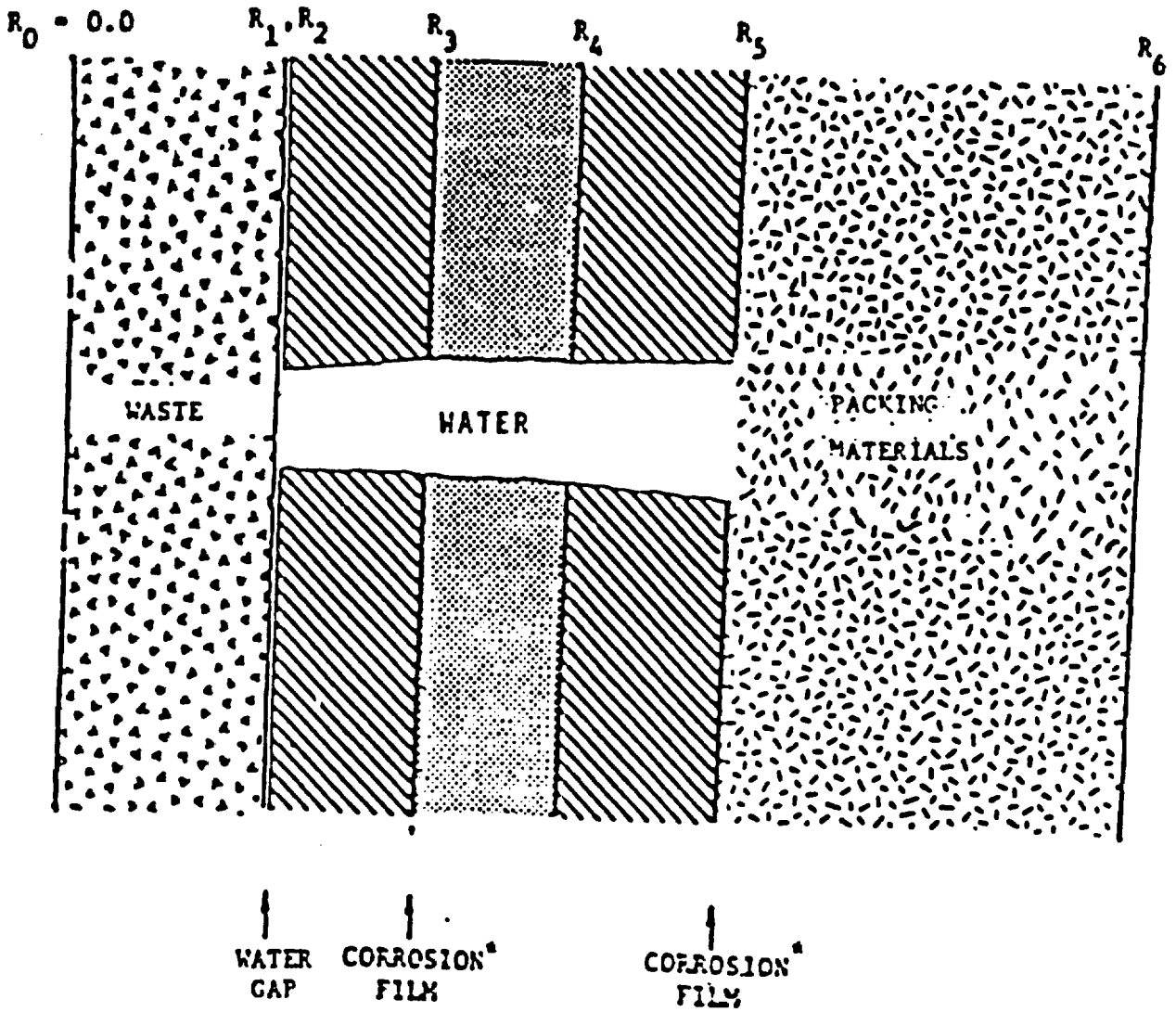
Provided the temperature is monotonically decreasing with time and neglecting the "improper" use of the temperature at the end of the time step to calculate oxide growth as previously mentioned, the solution procedure currently used by WAPPA for dry oxidation will overpredict the amount of corrosion. Although this approach is inconsistent from a physical viewpoint, it will be conservative.

2.4.3 Conclusions

The corrosion models used in WAPPA are intended to provide a conservative framework for estimating the degradation of the metallic barriers in the waste package. The modeling approach relies exclusively on user supplied empirical corrosion rates for each type of corroson process. These corrosion rates are generally supplied as a function of temperature only. The influence of other environmental parameters such as solution composition are not accounted for explicitly. Assurance that WAPPA's corrosion models are conservative requires that the input data can be shown to be conservative under any conditions expected in the repository during the containment period and the numerical solution procedure improved to calculate corrosion based on the maximum temperature during the time step.

2.5 WAPPA'S LEACH-AND-TRANSPORT MODEL (WMODEL)

With reference to Figure 2.4, the Leach-and-Transport Model is activated when all metal barriers have failed through one or more degradation mechanisms and the waste form is exposed to direct attack from the fluid flooding the breached barriers.



*Corrosion layer placed on the outer radius of the metal

Figure 2.4 Geometry of Waste Package
(adapted from ONWI-452)

The purpose of WMODEL is to calculate the release of radionuclides from the waste form, their transport out of the waste package, and the accumulated mass of each radionuclide delivered to the host rock. To that effect, the WMODEL relies on a leach submodel and on a transport submodel.

A description of the implemented modeling approach is provided in Section 2.5.1. A discussion follows in Section 2.5.2 Conclusions are drawn in Section 2.5.3.

2.5.1 Review of Modeling Approach

2.5.1.1 Leach Submodel

The leaching submodel is a leach rate expression which includes both dissolution and diffusion from the waste form and is modified by empirical correlations to account for the effects of temperature, radiation, solution saturation, and waste form fracturing. The implemented expression is:

$$Q_L = \left(\frac{1}{2}\, k_{dif} t^{-1/2} + k_{dis}\right) \cdot A_{FW} \cdot LEF \cdot SDENSF \left(1-\frac{C_{WM}}{C_{sat}}\right) \exp \frac{E(T-T_o)}{RTT_o} \quad (2.8)$$

where:

- Q_L = mass leach rate from waste form to solution (g/s);
- k_{dif} = leach rate coefficient for diffusion ($g/m^2\text{-}s^{1/2}$);
- k_{dis} = leach rate coefficient for dissolution ($g/m^2\text{-}s$);
- A_{FW} = total surface area of the waste form, including geometric and fractured areas (m^2);
- LEF = combined leach enhancement factor, the product of leach enhancement factors for alpha damage and γ-radiolysis as obtained in RMODEL (dimensionless);
- SDENSF = density degradation factor due to alpha damage as obtained in RMODEL (dimensionless);
- C_{WM} = concentration of the solute in the fluid at the waste form/canister boundary (g/m^3);

C_{sat} = saturation concentration of the solute (g/m^3);
T_o = reference temperature for k_{dif} and k_{dis} (°K)
E = activation energy (kcal/g-mole);
R = gas constant (kcal/g-mole-°K);
T = temperature of the waste form (°K).

The release rate depends on which species is being modeled as the two leach rate coefficients and the saturation concentration vary for each nuclide under consideration.

2.5.1.2 Transport Submodel

For modeling purposes and with reference to Figure 2.5, the WMODEL subdivides the cylindrical layered medium representing the waste package into three distinct regions: the waste form plus the fluid filled region extending to the first metal barrier, the flooded barriers, and the packing materials. The model further assumes that each species under consideration behaves independently from other species. Thus, given a particular species, one is left in general with solving a system of three coupled equations in terms of the concentration of the given species in the leachant next to the waste form, in the leachant within the flooded barriers, and in the pore fluid of the packing materials. In practice, however, the WMODEL solves a system of four equations which could be shown to reduce to one nonlinear ordinary differential equation. Proceeding from the waste form radially outwards, the reference equations of the WMODEL are as follows:

(a) The first equation describes the rate at which any selected species is transferred from the waste form to the contacting aqueous solution. This is Equation (2.8). It is the same for all species and it is the classical, diffusion and network-dissolution expression for the leach rate modified by a concentration-dependent, solubility limited factor and by further leach enhancement factors due to cracking of the waste form surface, α-damage to the waste form structure, and γ-radiolysis of the water. The dependence on

temperature is handled through an Arrhenius expression. In particular, the concentration profile within the water gap between the waste form and the canister is assumed to be uniform and to be controlled by diffusion processes taking place within the flooded barriers.

(b) The second equation couples the concentration of any given species in the water gap next to the waste form to the concentration of the same species at the interface between the flooded barriers and the packing materials. The concentration profile in this region is assumed to respond instantly to concentration variations at its boundaries and corresponds to a steady-state diffusion profile. Taking into account the layered, cylindrical geometry of the system, solution of the diffusion equation yields a concentration profile which drops logarithmically across the flooded barriers.

(c) The third equation computes a time-dependent, space-averaged concentration of a given species within the packing materials. This is accomplished by treating the packing materials as a mixing cell, i.e., the entering fluid is instantaneously mixed in the volume of the packing materials, and the concentration varies as function of time only. Any directionality of the flow field is lost in this approach, and convection in and out of the packing materials is handled through a leachant renewal frequency term. Diffusion in and out of the packing materials is difficult to justify in this approach. Nevertheless, a diffusion term, which has some directionality information, appears in the equation. In particular, diffusion out of the system is assumed to take place through a concentration gradient operating from the location of the log mean radius of the packing materials to their boundary with the host rock where the concentration of all species is assumed to be zero. Sorption on the packing materials is modeled through a constant retardation coefficient which slows transport out of the region.

(d) By continuity, the above space-averaged concentration of any species in the packing materials could be set equal to the concentration at the interface with the outer metal. This is not deemed, or recognized to be acceptable. Thus the fourth equation in the WMODEL relates the two concentrations through a proportionality constant defined as the ratio between the thickness from the log mean radius to the outer radius of the packing materials and the total thickness of the packing materials.

2.5.2 Discussion

2.5.2.1 Leach Submodel

Three major limitations have been found in the leach submodel. They are:

(1) The leach rate expression is not coupled with the radionuclide inventory in the waste form.

(2) The leach rate expression does not account for increasing radionuclide inventory under certain conditions.

(3) There is an inconsistency in the calculated mass released to the repository when the waste form is depleted.

Limitation(1)

The first limitation can be found through examination of the leach rate expression, Equation (2.8), which states that the rate of mass transfer from the waste form into solution is independent of the concentration in the waste form. According to this expression, the leach rate depends heavily on the diffusion and dissolution coefficients, k_{dif} and k_{dis}, which are to be determined empirically from experimental results and are specified in the code as input parameters which are constant with time. However, it can be shown theoretically[11] that both k_{dif} and k_{dis} are the product of the nuclide concentration in the waste form times a physical parameter that is process

specific. For example, the leach rate dissolution coefficient is the product of surface concentration, C(t), times the waste form dissolution velocity, u(t):

$$k_{dis} = u\ C(t). \tag{2.9}$$

Since the waste form concentration is a function of time due to leaching and radioactive decay, k_{dis}, as expressed in Equation 2.9, is also a function of time even if the dissolution velocity were constant.

To make the release rate a function of waste form concentration, k_{dis} and k_{dif} would have to be expressed as explicit functions of waste form concentration. However, WAPPA does not make any attempt to calculate waste form concentration. Thus, if the WAPPA model is to be retained, k_{dis} would have to be input as a time dependent function which reflects the changes in waste form concentration. This implies the user would need to estimate the waste form concentration as a function of time before performing the calculation. Similar remarks apply to k_{dif}.

As shown in References [12,13], the release rates of Cm-244 and Cm-245, as obtained from WAPPA's complex verification test case provide an example of the problems that can arise by not coupling the leach rate to the mass inventory in the waste form. Since Cm-244 and Cm-245 are isotopes of the same element, they were given identical leach rate coefficients in the test problem. Therefore both nuclides were calculated to be released from the waste form at the same rate, despite a 14-orders-of-magnitude mismatch in their initial inventories. In fact, WAPPA predicted all of the Cm-244 to be released from the waste form within the first second of leaching.

Furthermore, the nuclide concentration within the breached engineered barriers and the packing materials is a function of the nuclide release rate from the waste form. Thus, a consequence of unreasonably high leach rates is that calculated concentrations throughout the waste package are much too large and mass is not conserved.

For example, at 5600 years, which is the end of the first computational time step since the beginning of leaching, WAPPA calculates the average Cm-244 concentration as $5 \times 10^{-3} g/m^3$. However, the total inventory a supplied by the data base is $6 \times 10^{-16} g$. WAPPA does check whether the total mass released to the repository exceeds the current inventory in the waste form and it does prevent spurious mass from entering the repository. Nevertheless, it is wrong and misleading to calculate the concentration within the waste package as being so large that mass is not conserved.

Limitation (2)

The second situation in which WAPPA does not conserve mass occurs when the inventory of a given nuclide is increasing in time due to decay of other nuclides in the waste form. WAPPA calculates the release of each species until the mass released at a given time step equals the total mass found in the waste package. After this time, WAPPA assumes this species is completely and permanently removed from the waste form. WAPPA neglects to check for production of the species due to decay of other nuclides after the nuclide under study has been removed from the waste form. This approach is non-conservative and can underpredict the release of a nuclide into the repository. To clarify this point, the complex verification test case was run and the results for Th-229 (which does have an inventory that increases in time) mass release to the repository was examined.[13] WAPPA predicted that $2.6 \times 10^{-3} g$ of the Th-229 was released to the repository over the first time step since the onset of leaching. At this time, this was the entire Th-229 inventory. Therefore, WAPPA stopped calculating release of Th-229 and $2.6 \times 10^{-3} g$ remained as the total release to the repository. However, the inventory of Th-229 continued to increase reaching a value of 2.1g at the end of the calculation. Thus, there is a non-conservative discrepancy between the amount of mass in the system and the amount of mass in the repository.

Limitation (3)

The third problem occurs because WAPPA takes an inconsistent approach to mass conservation within the repository. In most cases, radioactive decay

within the repository is not taken into account. The output data for Tc-99 provides an example: after 10^6 years WAPPA predicts there are 435 grams of Tc-99 in the repository. However, part of the data base required to run WAPPA is the mass inventory that would exist if the waste form had been left undisturbed. In this test problem, the mass inventory supplied from the ORIGEN2 computer code for Tc-99 at 10^6 years is only 16.8 grams. The cause of this discrepancy is WAPPA does not account for radioactive decay once a nuclide has left the waste form. Thus, the Tc-99 which leaves the waste form when the inventory is high enters the repository and remains there. Neglecting radioactive decay provides a conservative estimate of the mass in the repository.

However, there is one exception when radioactive decay in the repository is taken into account. This occurs when the waste form concentration is depleted by leaching during a time step. In this case, WAPPA sets the amount of mass in the repository to the total available for leaching. This approach has the effect of accounting for radioactive decay in the repository and can lead to a decrease in the amount of mass in the repository. Pu-239 exhibits the results of this logic. After 10^5 years, the calculated release to the repository is 34.4 grams. At 2×10^5 years, the end of the next computational time step, the ORIGEN2 inventory of Pu-239 is 8.6 grams and it is all released to the repository. Instead of adding the 8.6 grams to the amount in the repository and thereby neglecting decay, the mass in the repository is set to the ORIGEN2 inventory of 8.6 grams. Provided the mass inventory is decreasing, accounting for decay in this manner will still be conservative. However, it is inconsistent.

In addition to the logic flaw identified above, the expression for the leach rate itself appears to be unrealistic, or very conservative, for species which exhibit large solubility in water, e.g., the alkalis. Indeed, the model predicts for these species an initial inverse-square-root-of-time law for the release rate followed by a constant release rate at longer times, which is contrary to experience at low flow rates. This however does not constitute a serious error unless alkali leach rates are used in the future for helping predict the groundwater chemistry.

2.5.2.2 Transport Submodel

Despite claims to the contrary, the WMODEL does not give a "realistic" credit to partially breached barriers for retardation of radionuclide transport. Indeed, as soon as the breach occurs, the waste form is assumed to become totally wetted and to release directly into the packing materials. The only attenuation of the leach rate comes from adjusting its concentration dependent term to reflect a logarithmic concentration profile across the flooded barriers. Since this correction is very small, the barriers do not play any meaningful retarding role. Thus, under the logic of the WMODEL, a marked decrease in leach rates occurs only when solution saturation limits, with a value typical of waste form/canister interface fluid, are approached in the packing materials. This conservativeness is probably unnecessary.

The treatment of radionuclide transport in the packing materials is also unrealistic. The mixing-cel' approach applies best to situations where flow is not laminar, and it breaks down when diffusion becomes the predominant transport mechanism. Since the case has often been made for the packing materials to reduce convection and to privilege diffusion, a space- and time-dependent equation for the concentration of any given species in the packing materials would be more adequate. This would also eliminate the problem of extrapolating a space-dependent concentration from a space-averaged one, as is presently being done. Nevertheless, the approach implemented in the WMODEL is conservative providing accurate parameters are fed into the model.

Another potential problem with the transport submodel involves retardation of solute transport in the packing materials which is handled by a constant retardation coefficient. As the groundwater percolates through the packing materials some of the nuclides become sorbed on the solid thereby slowing their transport. In dilute solutions, experiments indicate the distribution between the solid and liquid phases is constant and therefore retardation is constant. However, as the solution concentration increases this is often no longer true[14] and retardation decreases. Therefore, since the

solution will be near the solubility limits around the waste package, a constant retardation coefficient may not be justified everywhere in the packing materials.

Furthermore, the retardation coefficient is expressed in terms of an experimentally determined distribution coefficients K_d and before the retardation coefficient can be useful for WAPPA it must be shown that the K_d's used are relevant to the situation. In particular, current K_d measurements are obtained from single component tests. For example, the distribution of plutonium between the solid and liquid phases is measured in an experiment which has only plutonium in solution. In general, sorption is a complex phenomenon which depends strongly on solution chemistry. Therefore, single component tests may not be applicable to repository conditions which will contain all of the nuclides released from the waste form. A more detailed examination of the potential problems with using a constant K_d (and therefore constant retardation coefficient) coefficient can be found in Reference (15).

The numerical strategy implemented in the WMODEL appears to be too crude and error prone. In practice, the WMODEL solves a non-linear differential equation of the type:

$$\frac{dC_B}{dt} = f(t,C_B) \tag{2.9}$$

in terms of the space-averaged concentration of radionuclides in the packing materials, $C_B(t)$, during a time step (t_i, t_{i+1}), where $f(t,C_B)$ is a nonlinear function of time. The quantity $C_B(t)$ is related to the concentration at the outer surface of the metal, C_n, through a practically constant factor, b, comprised between 1 and 2 (Section 2.5.1.2):

$$C_n(t) = b\ C_B(t) \tag{2.10}$$

The concentration at the waste form-metal barriers interface, C_1, is related to C_B through the following relationship:

$$C_1(t) + C_n(t) + d \cdot (k_1 t^{-1/2} + k_2)\ (1 - \frac{C_1}{C_{sat}}) = b\ C_B(t) + d \cdot (k_1 t^{-1/2} + k_2)\ (1 - \frac{C_1}{C_{sat}}) \tag{2.11}$$

where d is a practically constant factor, and k_1, k_2 and C_{sat} are constants. The WMODEL solves the above problem by taking t in the RHS of Equation (2.9) and $t^{-1/2}$ in Equation (2.11) as constant over the time step, which is obviously a poor approximation if the time step is large. Thus, even if, with adequate data, the logic of the WMODEL would insure conservatism, one can not guarantee it until a numerical error analysis is made.

2.5.3 Conclusions

WAPPA's Leach-and-Transport Model is inadequate in that it does not conserve mass, does not couple the leach rate of a nuclide to the concentration within the waste form, does not even calculate the waste form concentration, and at times is inconsistent with its own assumptions. To properly repair the WAPPA model would require expansion of the current scheme of calculating four primary variables: leach rate, and concentrations in the packing materials, at the edge of the packing materials, and in solution at the surface of the waste form; to include a fifth variable: concentration within the waste form. Also, a global mass balance should be performed to insure that mass is conserved and that the total mass in the waste package/repository system is equal to the mass inventory supplied as input. To accomplish this would require a substantial part of WAPPA's leach-and-transport model to be rewritten.

As currently implemented in WAPPA, the Leach-and-Transport model will provide a conservative estimate of the release of any species from the waste package through the engineered barriers to the repository only if the mass inventory of a given species decreases with time and the accuracy or conservativeness of the input parameters and numerical solution can be assured. This cannot be done easily.

2.6 CONCLUSIONS

A common aspect to all of WAPPA's process models is that they involve an empirical approach at modeling the physico-chemical behavior of the waste package under expected repository conditions. A list of specific limitations of the modeling work in general and of the individual process models in particular is presented in Table 2.0.

The main shortcoming of the implemented modeling approach is that the process models are not self-standing, i.e., they imply a large number of assumptions and rely heavily on user-supplied inputs. For practical applications and acceptability of the results, it will behoove any potential user of WAPPA to make sure that all assumptions that went into the modeling are indeed warranted and that the data used are indeed relevant for each problem. Both tasks are significant as they may require comparison with more detailed analyses and initial information that is difficult to obtain from or it may not even exist in the literature. In particular, because of the recognized lack of pertinent data in the literature and the uncertainty associated with some of the data, it is unlikely that any two users will create the same data base.

An additional complication of the implemented modeling approach is that it requires a priori knowledge of the coupling between repository and waste package performance as temperature, pressure, and groundwater flow rate at the waste package-host rock interface as a function of time do depend on waste package feedback effects. At present it is not clear how this inconsistency can be solved.

A major omission in WAPPA's modeling approach is a groundwater chemistry model. The influence of groundwater chemistry on corrosion, leaching, and nuclide transport is assumed to be incorporated into the user supplied input. There is no provision for modeling the coupling between these processes and changes in groundwater chemistry. This places on the user the extra burden of showing that the selected data is indeed conservative under all expected groundwater compositions.

Table 2.0 Significant Limitations of WAPPA's Modeling

Model		Limitations
General	1)	Most models are empirical and extremely data intensive.
	2)	No explicit groundwater chemistry model.
	3)	Groundwater flow treated as a boundary condition.
	4)	No internal time step selection and error control.
Radiation	1)	Data requested for radiation damage models may be unavailable.
	2)	Radiolysis effects are independent of temperature, groundwater chemistry, and nuclide under consideration.
Thermal	1)	Temperature at the waste package/repository boundary is required as input.
Mechanical	1)	Materials strength is independent of temperature.
	2)	Expansion of corrosion products is neglected.
	3)	Failure of the waste package ends is neglected.
	4)	Data for empirical formulae may not be available.
Corrosion	1)	All corrosion processes depend only on temperature.
	2)	Data for pitting, crevice, and/or crack size and density may not be available.
Leach-and-Transport	1)	No global mass balance.
	2)	Leach rate independent of mass in the waste form.
	3)	Leach rate does not consider radionuclide inventory increasing due to decay of other nuclides.
	4)	Inconsistent approach in calculating mass released to the repository.
	5)	Leaching and transport retardation are independent of solution chemistry.
	6)	Data may be unavailable or difficult to obtain.

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3. REVIEW OF WAPPA'S OPERATION

As indicated in Chapters 1 and 2, WAPPA's modeling approach is more empirical than mechanistic, which places the task of preparing extensive data files to run the code for each problem at hand on the user.

In order to make it more clear how the code operates, user's input specifications to WAPPA are reviewed in Section 3.1. Output specifications are briefly touched upon in Section 3.2. Conclusions are drawn in Section 3.3.

The analysis presented hereafter is based on the code manual and the complex verification test case which accompanies the code. The test case will be referrred to as "the test listing".

3.1 INITIAL SPECIFICATIONS

3.1.1 Geometrical Configuration and Materials Specification

With reference to Figure 3.0 which shows the initial configuration of the waste package in WAPPA's Complex Verification Test Case, the waste package is always approximated by a cylindrical, axisymmetric set of concentric barriers. This permits a one-dimensional radial formulation with empirical corrections for end effects.

Proceeding from the inside of the waste package outwards, materials specifications are indicated by entering the material identifier and its outer radius. Materials identifiers are 3-digit numbers. They are used to locate the material properties in the data base for each barrier material.

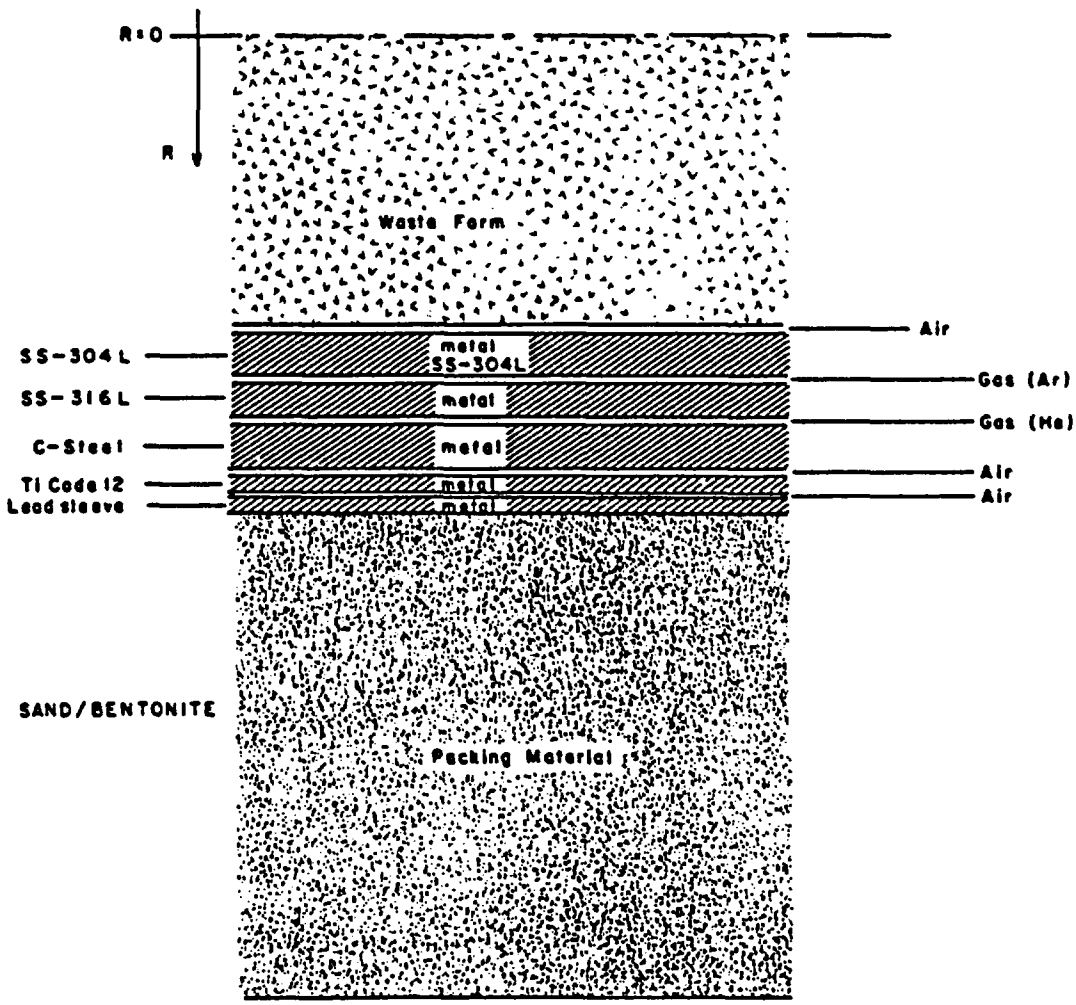

Figure 3.0 Initial configuration of the waste package in WAPPA's complex verification test case.

Allowable barriers are waste forms, metals, corrosion films, gases and packing materials. There can be 17 barriers at most; one waste form, one packing material, and five each of the other barrier materials. The materials reported in Figure 3.0 were inferred from Chapter 2 in the code manual. As a general comment, the test listing does not provide a key to the identification of each particular material constituting the waste package barriers. For instance the listing leaves one uncertain as to whether the waste form is glass or spent fuel.

Initially there will be no corrosion layer. Thus, WAPPA automatically assigns a zero thickness corrosion layer on the outside of each metal barrier. As a minor point, however, since WAPPA accounts for dry oxidation of metals, it would seem more consistent if, when applicable, corrosion layers could be placed on both sides of metal barriers.

The above information is complemented by inputting the waste package height, the volume fraction of the waste form which is waste, the density of the waste form matrix without the waste, the density of the waste, and the mass ratio of reprocessed waste-to-original fuel fed in the reactor. In particular, the listing does not mention the age of the waste. That has to be inferred by examining the power source decay rate.

3.1.2 Calculation Times and Error Control

In the preparation of the input to the code, the user must define the time span to be investigated along with a set of up to 400 time steps into which the analysis should be subdivided. A restart option also exists which allows restarting the program at any specified time point and continuing the analysis with a newly defined time-step vector.

In any numerical simulation of a time-dependent problem, the solution accuracy can be enhanced, while retaining efficiency, by selecting a time step that is small when changes are most rapid and increasing the time step when the rate of change decreases. In modeling waste package performance, the time

when changes are going to be most rapid are initially when the heat source decreases most rapidly due to the decay of short-lived radionuclides, and, at later times, when breaching of a barrier occurs allowing the groundwater to contact the next barrier. Since the user specifies the time step through an input table containing all of the time steps, WAPPA does not determine the time step consistent with the physical processes that occur. This can lead to large, although conservative, errors in the calculated times of breaching and onset of leaching. For example, if the calculation showed the barrier adjacent to the waste form will breach between the requested computational times of 1000 and 1500 years, leaching would be assumed to begin at 1000 years.

To define the temporal location of barrier failures more precisely, the calculation must be repeated with a finer subdivision of computational times. WAPPA can facilitate this process through the restart option. Using the previous example, to determine the onset of leaching within a 50 year period, the calculation could be restarted at 1,000 years requesting a computation every 50 years between 1,000 and 1,500 years. This procedure is a cumbersome burden to the user which could have been avoided by incorporating some time step selection logic into the computer code.

Furthermore, the lack of error control during the calculation prompts the question of how accurate is the solution. The only method the user has to determine if the solution has converged is to rerun the code several times using a finer time discretization for each new run and comparing the results. Again, this is a burden to the user which could be resolved by proper checks within the computer code.

3.1.3 Nuclides Requested

The user is required to specify as input the radionuclides to be tracked during a particular computation. Each radionuclide is identified by a five digit number representing the radionuclide's atomic number and its atomic mass. Thus, 43099 is Tc-99 and 93237 is Np-237. As an added feature each nuclide is also reported in the test listing using the element symbol and its atomic mass.

Since any number of radionuclides can be selected provided a data base for each of them exists, the code tacitly assumes that all radionuclides behave independently from each other. This can be a limiting assumption for nuclide leaching and transport. Thus, the user must make sure that leaching and transport data for each radionuclide were taken from a complex interaction test where all species were allowed to react with each other and with the waste package barriers.

3.1.4 Repository Boundary Conditions

In order to account for waste package interaction with the near field of the repository the user must supply WAPPA with the temperature, fluid flux, vertical stress, and radial stress at the waste package-host rock interface as function of time. The user must also specify packing materials resaturation time.

Singling out the waste package-host rock temperature, one must reason that it depends, as a function of time, both on repository properties such as rock thermal properties, area thermal load, waste package arrangement, etc. and on intrinsic waste package properties such as waste package dimensions and heat generation rates. Thus, in order to specify the problem, it would seem that one needs to have solved it before hand. The same is true for packing materials resaturation time, fluid flux, and, to a lesser extent, for the repository confining pressures.

Boundary conditions specification is one of the most limiting problems in the use of WAPPA, as the above quantities do depend on waste package feedback effects. The problem might be solved by attempting to develop simplified near- and far-field models and interface them with WAPPA.

3.1.5 Data Base

WAPPA's basic modeling approach is empirical in nature and therefore extemely data intensive.

Data needed in order to operate the code include radiation decay properties, radiation shielding properties, empirical data for radiation damage, thermal properties, mechanical properties, empirical data for end effects on stress analysis, empirical data for corrosion, empirical data for leaching. Some of these data need to be supplied as function of waste package system variables like temperature, pH, etc.

The task of assembling such a large data base can be overwhelming for several reasons. First, the user must be thoroughly acquainted with the limitations and the range of applicability of the implemented models. He should also be able to judge whether the data do exist in the literature. If the data are not available, ad hoc experiments and/or extensive calculations are needed. Because of the paucity of the data and uncertainty in some of the data, it is unlikely that any two users will create the same data base. The second problem is that the range of experimental data to be inserted in the data base should cover the entire history of the waste package under expected repository conditions. The waste package environment and physical barriers can vary so extensively during the time span of a repository that it is hardly conceivable that an adequate data base where all synergistic effects are accounted for can be produced. For instance, the Corrosion Model uses empirical correlations to supply all information regarding corrosion rates for each of the various models and barriers. The coefficients used in each correlation are supplied by the code user as a function of temperature alone. One would expect corrosion to depend also on pH, Eh, salts content of the groundwater, etc. which readily increases the complexity of the problem of obtaining adequate experimental data. It is forseeable that the user of WAPPA shall not model all synergisms and will refer to single or few-component test data. In that case, the user will have to show that these data are conservative.

3.1.6 Radionuclide, Gamma, Alpha, and Thermal Power Source Terms

At each new time step WAPPA updates the radionuclide inventory and the thermal-power, gamma-photon, and alpha-particle densities in the waste form through usage of user-provided input tables. These tables are prepared by running beforehand an isotope inventory code like ORIGEN.

The task of preparing the above inputs is not onerous to the user as it requests that only the age and type of waste be known. Barring numerical errors due to WAPPA's lack of internal time step and numerical errors controls, this implemented approach is conservative, as the source term code would not account for radionuclide depletion with time from the waste form due to leaching and transport.

3.2 OUTPUT SPECIFICATIONS

WAPPA allows many options to control the amount of data to be printed. Options exist for echo prints of the input a well as the output of results generated during execution. Always provided are the total radial heat flow leaving the waste package, the cumulative γ-radiation dose, nuclide fluxes at the waste package boundary, total nuclide mass outflow through the waste package boundary, radial nuclide concentration, profile in the waste package,- barrier wetting times, and barrier failure times.

The output to the code reads well. It requires however some familiarity with the code structure and how it operates. As a general comment we would suggest that the output be improved to show 1.) The name of each material being considered rather than only a numerical identifier, 2.) The mode by which a barrier may have failed, and 3.) Whether mass is conserved or not in the system. Additional minor points are the following: 1.) The leach rate diffusion and dissolution coefficient are given wrong dimensions; 2.) Dimensions are missing from the oxidation rate constants A through G; and 3.) On restart runs the radionuclide mass inventory, alpha flux, and gamma flux are given wrong dimensions.

3.3 CONCLUSIONS

The operation of WAPPA involves the preparation of extensive input and support data files. These should be prepared by qualified personnel who are thoroughly acquainted with the assumptions which went into the formulation of each process model.

The task of preparing input and support data files can be overwhelming for two main reasons. First, some of the input data require a pre-knowledge of how the waste package would perform. Second, the amount and quality of the needed data contrasts with the recognized paucity of pertinent data in the literature and their associated uncertainty. To that effect, it should be mentioned that WAPPA users will probably be limited to data which factor in only a few of the system variables on which they depend. Thus, it will be necessary for any WAPPA user to show that these data are conservative.

WAPPA's implemented numerical strategy lacks internal control of time step and of numerical errors. This may lead to unnecessary conservatism and place on the user the extra burden of redefining the time step vector and re-running the code several times in order to make sure that convergence is achieved. This feature, along with the large number of data whose uncertainty needs to be known, limits WAPPA's applicability for Monte-Carlo-type reliability analysis, which requires short computational time for each case run.

4. CONCLUSIONS AND RECOMMENDATIONS

4.1 CONCLUSIONS

WAPPA is a modular code implementing radiation, thermal, mechanical, corrosion, and leach-and-transport modeling to determine system performance of high level nuclear waste packages in groundwater saturated porous media. The code logic is conservative and the modeling level is kept simple, as expected in a system code.

WAPPA was not designed to be a self-standing code. It implements a mostly empirical approach requiring model justification, and extensive data gathering, interpretation and validation. These tasks constitute the major limitations of the code and will require a significant effort to resolve by personnel who are thoroughly familiar with the modeling.

In practice, WAPPA operates as a data base manager that simply selects which correlation and which data are applicable for each particular situation. Construction of the data base will be troublesome as the implemented correlations may be defined in terms of only a few variables, whereas the actual processes may depend on more system variables; the required data are likely to be unavailable in many cases or they may be difficult to adapt from the literature; or they may imply a pre-knowledge of future package performance, as is the case for temperatures, pressure, and groundwater flow rate at the waste package/host rock interface. Furthermore, as reported in Table 4.0, a few limitations have been identified in the process models.

The number of parameters which will have to be supplied and the number of different situations for which they may have to be specified will result in very large data files. After formation of these files, the user must make sure that the adopted data base is realistic or conservative for the problem under study. The code user will also have to prove that all assumptions that

Table 4.0 Significant Limitations of WAPPA's Modeling

Model		Limitations
General	1)	Most models are empirical and extremely data intensive.
	2)	No explicit groundwater chemistry model.
	3)	Groundwater flow treated as a boundary condition.
	4)	No internal time step selection and error control.
Radiation	1)	Data requested for radiation damage models may be unavailable.
	2)	Radiolysis effects are independent of temperature, groundwater chemistry, and nuclide under consideration.
Thermal	1)	Temperature at the waste package/repository boundary is required as input.
Mechanical	1)	Materials strength is independent of temperature.
	2)	Expansion of corrosion products is neglected.
	3)	Failure of the waste package ends is neglected.
	4)	Data for empirical formulae may not be available.
Corrosion	1)	All corrosion processes depend only on temperature.
	2)	Data for pitting, crevice, and/or crack size and density may not be available.
Leach-and-Transport	1)	No global mass balance.
	2)	Leach rate independent of mass in the waste form.
	3)	Leach rate does not consider radionuclide inventory increasing due to decay of other nuclides.
	4)	Inconsistent approach in calculating mass released to the repository.
	5)	Leaching and transport retardation are independent of solution chemistry.
	6)	Data may be unavailable or difficult to obtain.

went into modeling are warranted. This will involve a detailed comparison of predictions from each process model with experimental results or with the predictions of state-of-the-art individual codes for each of the processes considered. In particular, since individual validation of each process model neglects the synergistic effects that may couple various processes, simultaneous validation of several models should be done whenever possible.

After validation of the data and models, the code user still must insure that the numerical solution procedure provides reliable calculations. At present, time step selection is determined from a user supplied input table which does not necessarily reflect the physical processes that occur, such as the breach of a barrier. Therefore, to insure the calculation is converged, the user must first run the code and determine the approximate times of major system changes. Then, the code must be rerun with a finer time discretization near the times of major system changes. This procedure must be repeated until the desired level of convergence has been achieved.

While adherence to the above procedures for code usage will be necessary for a license application, their rigor may be relaxed for work in site screening, preliminary design analysis, and in estimating acceptable ranges of parameters through sensitivity analysis. In this case, it may turn out to be profitable to use WAPPA once a few improvements have been made, e.g., mass conservation should be fixed in the leach-and-transport model, the temperature boundary condition could be given through a simplified far-field model, etc. All together these improvements may require a significant effort.

WAPPA cannot be used in its present form for straightforward reliability analysis, e.g., Monte Carlo simulation through Latin Hypercube sampling. There would be too many parameters to be sampled and probability distributions for all of them would not be available. Sensitivity analysis may alleviate the task by reducing the number of parameters to be sampled. However, the need to rerun to code a number of times to insure convergence may still prove a stumbling block for the reliability analysis both in terms of computer time and trouble to the user.

4.2 RECOMMENDATIONS

1. The WAPPA code is receiving considerable attention from the DOE's Salt and Tuff programs[3]. For this reason, the NRC should keep the code readily operable in its most recent form.

2. If the DOE decides to use WAPPA to obtain relevant licensing information, the NRC should request the code custodian to prepare an extensive data preparation manual which includes: a list of all the data required; a description of how the data is used; a description of model limitations; a list of appropriate references for obtaining the data; and a detailed example of how to construct the data base.

3. Any application of WAPPA should be complemented with an extensive justification of the data. Data should be prepared in accordance with the "Draft Technical Position on Waste Package Reliability".[1] That is, an estimate of the experimental errors the data should be presented along with a description of experimental procedures and a citation to the original reference.

4. Further work by the NRC using WAPPA does not seem to be justified unless the DOE indicates it will use the code to obtain relevant licensing information. In that case, an effort should be made to improve upon the present modeling approach of specifying the waste package/repository boundary conditions as a user-supplied function of time. For example, WAPPA could be coupled with a temperature field analysis which calculates the required boundary temperature as the calculation proceeds. Also, the various process models should be improved to remove their internal limitations. In general, model validation will be of primary importance.

5. If the NRC desires to have the capability to independently check-waste package performance calculations, it will need, in addition to a general systems code like WAPPA, a suite of state-of-the-art analysis codes that model the various individual processes that are

relevant. Examples of these processes include: groundwater flow, groundwater chemistry, heat transport, structural analysis, leaching, nuclide migration, and corrosion.

6. In the future, code manuals which provide a description of the mathematical and computational models should be prepared in accordance with the "Draft Technical Position on Documentation of Models."[2] In particular, the WAPPA manual, in many cases, did not provide adequate justification of the models, did not discuss the range of validity of the models, and did not address the problem of numerical stability and accuracy.

7. In the future, it would greatly assist the NRC if, in the code manual, the DOE provided a list or diagram of failure modes addressed by the code. Indeed, the preparation of a system code like WAPPA should be preceded by a failure mode and effects analysis (FMEA), in order to insure that all relevant failures are incorporated in the code. If available, this FMEA should at least be referred to in the code manual.

8. Although the modular structure of WAPPA would allow retrieval and re-adaptation of each process model to another code with a modular structure, this does not appear to be advantageous at present in view of the several shortcomings identified within each of WAPPA's process models.

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