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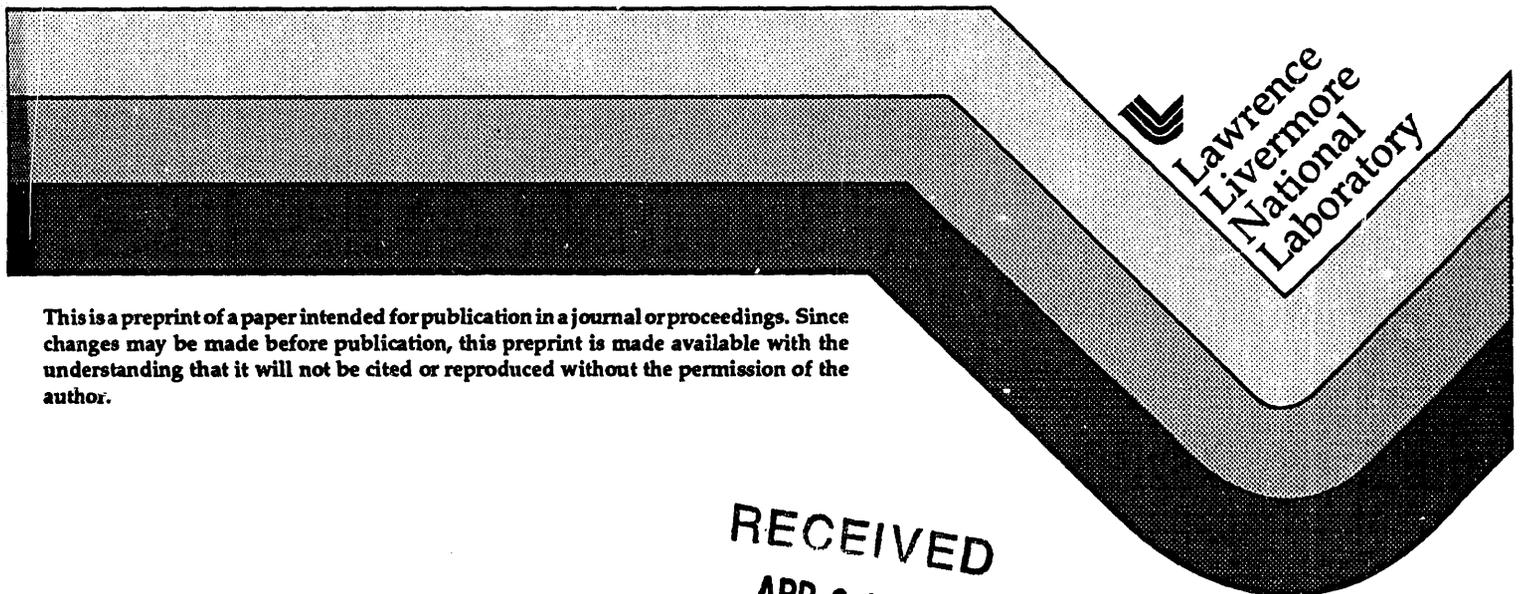
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Integrated Modelling of Near Field and Engineered Barrier System Processes

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INTEGRATED MODELLING OF NEAR FIELD AND ENGINEERED BARRIER SYSTEM PROCESSES

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ABSTRACT

The Yucca Mountain Integrating Model (YMIM) is an integrated model of the Engineered barrier System. has been developed to assist project managers at LLNL in identifying areas where research emphasis should be placed. The model was designed to be highly modular so that a model of an individual process could be easily modified or replaced without interfering with the models of other processes. The modules modelling container failure and the dissolution of nuclides include particularly detailed, temperature dependent models of their corresponding processes.

I. INTRODUCTION

The Engineered Barrier System (EBS) includes the containers for the waste packages, the waste form, and the emplacement mode of the waste packages. Evaluating the waste isolation capacity of the EBS requires modelling these components and estimating the corresponding physical and chemical parameters of the models. Considering that both model development and parameter estimation can be a costly and time consuming activity, management of the process at LLNL required a tool for identifying areas where research resources should be placed. Specifically a tool was needed to identify those components and processes where simple models and/or approximate estimations would be adequate, and those areas where more sophisticated models and accurate estimates are required. YMIM was developed as a flexible test bed to help us identify areas for emphasis. It has also been extended to

provide a source term model for larger modelling efforts.

A single run of YMIM models the releases from a set of waste packages that are all subject to similar temperature, hydrologic, and geochemical conditions. Although all of the packages are subject to similar conditions, there is variability in their releases because it is not assumed that they fail at the same time. Due to statistical variability in the maximum corrosion rates between packages, the packages fail at different times and will release nuclides at different rates. To model all of the packages in a repository, which would be subjected to a range of temperatures, hydrologic conditions, and geochemistry conditions, several runs of YMIM are made and the results added together.

Although the EBS may be limited to the waste package and its immediate surroundings, the performance of the EBS is strongly influenced by the temperature, hydrology, and geochemistry at the repository horizon. These, in turn, are influenced by engineering decisions about waste package placement, fuel age, and areal heat loading. YMIM has been designed to take these considerations into account in its analysis. However, in the current version of YMIM hydrology, temperature and geochemistry are not modelled internally. Rather, YMIM uses scenarios over these phenomena generated by other models.

The remainder of this paper will first discuss the philosophy that was followed in designing and developing YMIM. Then the structure of YMIM and the way it has been

implemented are described. Finally, we discuss recent extensions to YMIM and future directions.

II. THE DESIGN PROCESS FOR YMIM

YMIM allows investigators to study the sensitivity of releases to both variations in systems parameters and to variations in system models. To do this YMIM had to have two basic properties: First, it had to be an integrated model. As an integrated model it can estimate the impact that variations in models and parameters have on the releases from the waste packages. Studying the sensitivity of component processes by themselves to changes in parameters is not sufficient, since it is the actual releases that are important and the interaction with other processes might amplify or attenuate the impact of one process. Second, the structure of YMIM had to be flexible so that models of individual processes could be changed easily without disrupting, or invalidating, the rest of the model structure.

Setting up the structure of the computations was the first design decision in developing YMIM. For the processes in YMIM it was recognized that the calculations can be adequately made on a period-by-period basis. The state of all the process is given at the beginning of the period. Then the model directly calculates the change in state of each process during the period. This gives the state at the start of the next period. This approach contrasts with some other performance models such as models of temperature and hydrology which may require several iterations of calculations to solve their governing equations.

Structuring the calculations this way does lead to some small compromises in cases where two interacting processes go on simultaneously. For example, the wetted area of fuel rods depends on the amount of the fuel rod that has dissolved, and the amount that dissolves depends on the wetted area. In principle, these two processes interact during a period. However, under this computational structure it is assumed that the wetted area of the rod stays constant during a period. It can be updated at the end of a period when the amount dissolved during the

period is calculated¹. These compromises can lead to small errors which can be reduced by using shorter time periods, if desired.

Defining the processes to be included was the next step in designing YMIM. There are really two issues here. First, the processes need to be identified—basically this step just names the processes to be included and provides the fundamental organization of the model into processes. Then each process is further defined by describing exactly what its scope will be and how its internal processes will be modelled. Although there are only a few natural ways to divide the problem into separate processes, there is no single, unique way. We chose to divide the problem into the following major processes:

- near field chemistry: the chemistry of the groundwater reaching the containers and reacting with the waste form,
- near field hydrology: the fluxes at the repository horizon and frequency of episodes during which fluxes are flowing or the rock near the waste packages is wet,
- container failure: corrosion and failure of the waste package,
- cladding failure: failure of the fuel rod cladding through temperature creep and hydride reorientation in the fuel rods and through attack by fluorine in groundwater,
- nuclide behavior: rates of decay, and solubilities,
- rod and container temperature: temperatures of the waste form and the surface of the container,
- rock to container flow: movement of groundwater from the rock to the container taking into account any packing materials.
- internal container flow: flow of water over the waste form and the wetting of area on

¹ In the current version of YMIM an even simpler model of wetted area is actually used.

the fuel rods where the cladding has failed, and

- waste form dissolution and accounting: accounting for all of the material that has been altered, dissolved, and decayed.

These processes were studied by different groups of researchers at LLNL. The definition of the processes does not exactly map onto the organizations of the groups. Part of the process of defining the processes was identifying the researchers working in each area.

Simply identifying the processes did not define them as precisely as was required for the modelling effort. The final definition was developed based on the definition of the *interfaces* between them. Thus the modules are defined in YMIM in terms of the information that they are required to provide to other modules. Defining the modules this way ensures that they are independent of each other and they can be modified without disturbing other modules: as long as a new module provides the information expected of it, and it makes its computations using the period-by-period updating described above, its internal structure is not critical to the functioning of YMIM as a whole.

The interfaces were defined by interviewing researchers in one area about the information that they required from other areas in order to make their own calculation. For example, the model of alteration requires information about rod temperature and the exposed, wetted area of a rod. Through a series of interviews, we established the full set of information required for modelling each process. The information requirements were assigned to each process. Figure 1 shows the modules and the information that each module is expected to provide. The arrows between the modules show the actual communications between modules (although in principal any module can call any other module for information).

The model within each module could then be developed knowing what information it was expected to provide, and the information that it could expect to be available from other modules. For the initial version of YMIM a fairly simple model was designed for each process. A

computer program module was then developed for each process.

This approach simplifies the model construction and it simplifies the process of extending YMIM. The initial modules were fairly simple representations of their corresponding processes. Since the initial development of YMIM more complex modules using more sophisticated modelling have been substituted. As long as a new module can produce the information defined for that process, it will work in YMIM.

Modularizing YMIM and standardizing the interfaces this way also makes it convenient to use different versions of a module. This might be done in order to substitute a smaller faster running module for a slower module. It is also needed because some of the modules are expected to model different situations. For example, a version of the Dissolution and Accounting module can be written to model glass waste forms. This can be substituted for the current module which models reactor fuel assemblies.

III. IMPLEMENTATION OF YMIM

Because YMIM is structured around modules and these modules exchange information, it is natural to implement it using an object oriented language. C++ was selected because it has all of the features that were needed for YMIM and is available on a wide variety of machines. YMIM is currently implemented on both the Macintosh and the Sun.

The computer program consists of a main driving routine and the set of modules which are implemented as objects². When a run of YMIM is started, the main driving routine is executed

² In an object oriented language, an "object" is a module of the program that includes its own data and a set of subroutines that can operate on the data. One module can call another and instruct it to execute one of its routines. The routine might cause the object to initialize itself by reading data from a file, or it might instruct the called object to compute an answer and pass it back to the calling object.

first. It creates the objects for each of the modules and instructs them to initialize themselves. During initialization a module reads its data from its own data file and makes any initial computations and variable assignments it needs.

After initialization the main driving routine steps through the periods of the run. Each period it instructs the Dissolution and Accounting Module to compute the releases that period. To make this computation the Dissolution and Accounting module updates its internal state and calculates the releases. However, doing so requires information from several other modules. It passes messages requesting the needed information to the modules that can supply it. When they receive this request, the other modules update their internal state for that period and request whatever information they need from still other modules. This chain of calls continues until the modules that simply provide scenarios are reached. These return the values needed and each module along the chain can then complete its calculation.

At this time, each module reads its parameters from its own data file. New versions of a module may require more, or different, parameters than the module it replaces. By letting each module read from its own data file, we avoid the problem of restructuring the data files each time a module is modified. However, the specification of the structure of the data file must be included in the specification of a new version of a module.

IV. DESCRIPTION OF THE PROCESS MODELS IN YMIM

The process models in YMIM were initially developed using fairly simple assumptions. As YMIM has been applied to new questions, several of the modules have been extended to include more complex process models. Table 1 summarizes the modelling approaches currently used by each module.

While most of the modules include a model of their processes, the Hydrology, Temperature, and Near Field Chemistry modules simply

provide scenarios for the other modules. Their states at each period (i.e. the rod and container temperatures and the fluxes in the near field rock) are read in from their data files. At each period they make this information available to the other modules (although they do some simple interpolations). These scenarios are calculated from other models outside of YMIM. Because these are calculated external to YMIM, the user must ensure that the scenarios are consistent (i.e. the temperatures used must be consistent with the fluxes assumed).

The Container Failure and the Dissolution and Accounting modules contain the most detailed modelling in YMIM at this time. The paragraphs below describe the models in these two modules in more detail and the way that they interact with other modules.

A. Container Failure Module

The container failure module can model the corrosion of single and double walled containers. It includes temperature dependent models to account for dry oxidation, general aqueous corrosion, and localized (pitting) corrosion of the container materials. For each wall the user can specify the corrosion mode to be applied.

The dry oxidation and general aqueous corrosion models use deterministic, temperature dependent corrosion rates. Typically these are used to model the corrosion of mild steel container walls.

The localized corrosion model is typically used to model the corrosion of stainless steel container walls. It is a probabilistic model that estimates the fraction of the container walls that fail due to pitting corrosion each period. This model is based on a stochastic pitting model developed by Henshall, et al. Under this model, it is assumed that a number of pits will form on the surface of a container with varying depths. A container will fail when the deepest pit penetrates the thickness of the container wall. The fraction of containers that have failed in any given period is equal to the probability that the deepest pit on a container is deeper than the wall thickness.

Figure 1

The modules can provide all of the data listed to any module that requests it.
The primary data flows are shown as arrows.

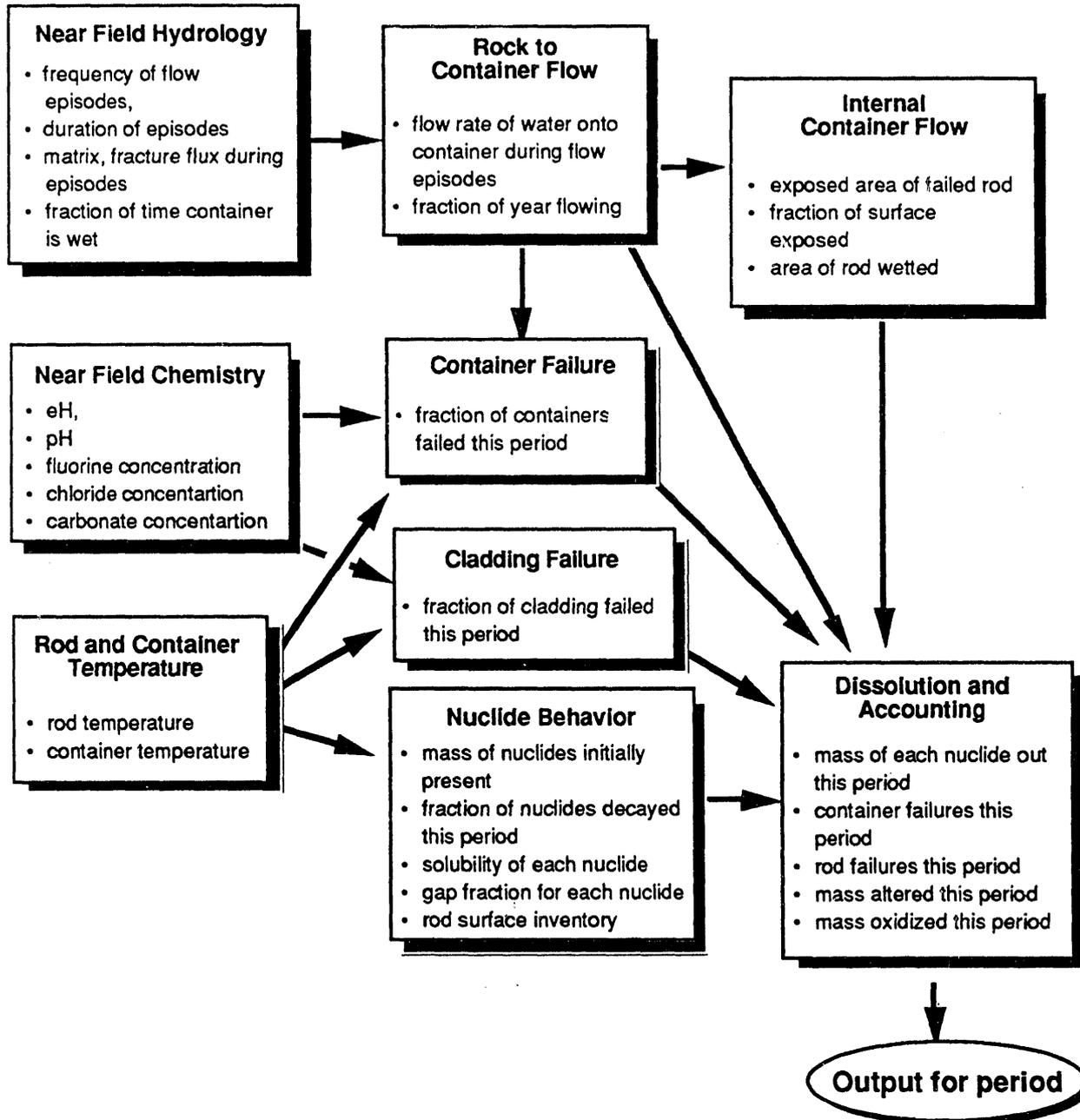


Table 1
Summary of Process Models Included in YMIM Modules

<u>Module</u>	<u>Approach</u>
Near-field hydrology	Time history of matrix and fracture flux in rock past package
Rock to container flow	Flux collection area converts flux in rock to flow directly into container
Near-field chemistry	Time history of pH, eH, chloride concentration, carbonate concentration, and fluorine concentration in groundwater
Temperature	Time history of container-wall temperature and fuel-rod temperature
Internal container flow	Estimate of exposed and wetted area of rods with failed cladding is based on the assumption that failed fuel rods are split due to oxidation of fuel
Container failure	(Described below) Temperature dependent models of air oxidation, general aqueous corrosion, and pitting corrosion; Early failure of defective containers and user specified failures
Cladding failure	Cladding fails due to creep rupture and hydride reorientation when rod temperature is in critical ranges; Cladding fails due to fluorine in groundwater.
Nuclide behavior	Solubilities of nuclides are temperature dependent; Each nuclide is assumed to decay according to its half-life, independent of the other nuclides.
Dissolution and accounting	(Described below) Fuel-matrix alteration and oxidation, and nuclide dissolution are temperature dependent; Pulse release from fuel-cladding gap; Gaseous nuclides are released from fuel cladding; Total releases are accounted for to ensure that max release is less than total present.

Since a container is failed by the deepest pit on its surface, the model develops a probability distribution over the depth of the deepest pit on a container. This distribution is known as an "extreme value" probability distribution. The complementary cumulative of the extreme value distribution, evaluated at a depth of X, gives the probability that the deepest pit on a container is deeper than X. When X is set equal to the

container wall thickness, complementary cumulative gives the probability that a container has failed. By computing the extreme value distribution over pit depth at each period in the model run, YMIM estimates the fraction of containers that have failed at that period.

B. Dissolution accounting model

The dissolution and accounting module models the dissolution of failed rods and

accounts for the mass of each nuclide that is released. The dissolution rate estimate is determined by two temperature dependent processes, the rate at which nuclides are freed from the fuel matrix by either aqueous alteration or dry oxidation, and the solubility of nuclides in water flowing over the exposed area of failed fuel rods. This module keeps track of the total dissolution in containers to ensure that the dissolution does not exceed the amount of material that is actually exposed to dissolution processes. Finally, the module accounts for the total decay of each nuclide.

Since the alteration and dissolution of fuel rods can only start once the package has failed, this module keeps track of the fraction of packages that fail in each period. It groups all of the containers that fail in one period together and models their subsequent history of fuel rod alteration and dissolution separately from other groups. At each period it sums up the releases from all of the groups that have failed at or before that period.

Upon failure of the package, it is assumed that air will come in contact with the failed rods leading to oxidation. Oxidation is modelled as a temperature dependent process. If water is present, it is assumed to be in contact with part of the exposed surface area of the rods. The size of the exposed and wetted surface area is modelled by the Internal Container Flow module. The rate at which the wetted fuel matrix is altered is dependent on temperature and water chemistry. Water chemistry data is provided by the Near Field Chemistry module.

The masses of nuclides in the matrix that has been altered each period are available for transport. The amount of each nuclide that is actually dissolved and transported away is determined by its solubility which is a function of rod temperature. Nuclides with very high solubilities ("alteration limited") are entirely dissolved and transported away as they are released from the matrix. Other nuclides only dissolve to the extent possible each period. The module keeps track of the total amount of each nuclide that has been released from the matrix, but not yet dissolved and transported each period.

V. Future directions

YMIM has been used as the source term model for the 1993 Total System performance Analysis (Wilson et al). It has also been used to study the effects of various temperature sensitive processes in the EBS (see companion paper by Gansemer and Lamont "Identifying Significant Uncertainties in Thermally Dependent Processes for Repository Performance Analysis").

In the future it is expected that several of the modules will be extended further, particularly those that model the fuel dissolution processes. We are also developing a formal system for version control and documentation to handle multiple versions of the software developed for different purposes.

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