

Modeling Disruptive Events Using the β -SOAR Model: Levels of β -SOAR Model Flexibility in Applications and Initial Insights

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The U.S. Nuclear Regulatory Commission recently developed a generic analytic model, β -SOAR (beta Scoping of Options and Analyzing Risk) that is intended to provide insights into an efficient and effective regulatory program for high-level radioactive waste disposal. β -SOAR is capable of modeling generic repository systems without disruptive events. However, flexibility is built into the model to simulate these events. The objectives of this paper are to identify limitations to this flexibility and determine future model development needs for disruptive events. In this paper, the frequency and magnitude of seismic, disruptive events are modeled by a Poisson process, with peak ground velocity correlated to waste package mechanical damage. Experiments with β -SOAR indicate that large but rare disruptive events can be modeled in a straightforward manner. For disruptive events of lesser magnitudes and higher frequency, model component modifications are required. The results suggest that research in backfill integrity, waste package material damage mechanisms, and seismic-induced stress corrosion cracking models may provide further risk insights.

I. INTRODUCTION

It is likely that discrete, disruptive events may impact geological disposal systems aimed for long term isolation of high-level wastes (HLW) and spent nuclear fuels. Since the early days of geological disposal system planning and investigation, policy and decision makers have considered disruptive events caused by seismic and tectonic processes an important factor for developing safety standards and goals¹ or to siting potential geological repositories². More recently, performance assessments for planned or potential geologic repository systems by the Swedish Nuclear Fuel and Waste Management Co.^{3,4} and for the proposed high-level waste repository at Yucca Mountain by the United States Department of Energy⁵ consider the potential impacts of seismic features and events on repository performance. Disruptive events such as volcanism, fault displacement and deformation of geological formations resulting from

seismicity are considered in other countries, e.g., Japan⁶, where tectonic stability is an issue. Earthquakes or seismic events might result in fault displacement or failure of embedding structures such as tunnels, boreholes or drifts. Depending on the design of the disposal system and its interaction with the natural geologic formations, waste packages may sustain various degrees of mechanical or dynamic damage as a result of seismicity.

The occurrences of individual disruptive events are unpredictable. Their magnitudes and impacts to geological disposal systems and the embedded high-level wastes and waste packages cannot be assessed deterministically. The aleatoric and uncertain nature of disruptive events also poses challenges to mechanistic and process-level models that attempt to identify and simulate the failure mechanisms of the engineered barriers in geological disposal systems. Additionally, experimental and modeling efforts regarding mechanical waste package damage are limited to a small number of proposed waste package materials.

In an effort to provide insights into the development of a more efficient and effective regulatory program in response to potential changes in the U.S. high-level waste policy, the U.S. Nuclear Regulatory Commission (NRC) recently developed a simplified generic analytic model named β -SOAR (beta Scoping of Options and Analyzing Risk). A disruptive events component was recently developed and tested to enhance β -SOAR's capability. This paper describes a disruptive event prototype model of β -SOAR, highlights model development, knowledge and data needs, and potential challenges in providing meaningful input to the U.S. NRC's high-level waste regulatory program.

II. APPROACHES

The β -SOAR model was developed by incorporating selected, key features, events and processes (FEP) that provide a simplified representation of five model components common to most geologic disposal systems: waste form, waste package, near field, far field and

biosphere. A component model was recently developed and integrated with the β -SOAR code, to assess the impact of disruptive events to the performance of selected, generic geologic disposal systems. At present, because of the lack of candidate repository sites and the generic nature of the β -SOAR code, the implementation is abstractive. The implementation of FEP's related to disruptive events and mechanical waste package material damage is similarly abstractive. In particular, abstractions of waste package emplacement design, e.g., tunnel vs. borehole, selection of backfill materials, waste package size and shape, waste package damage or puncture mechanisms, and waste package thickness evolution as affected by local and general corrosion have not been explicitly expressed in the implementation of the β -SOAR disruptive event model prototype.

II.A. Seismic Events

Seismic events may be assumed to follow a Poisson process, with a pre-determined mean event frequency. A Poisson distribution is a probability distribution that characterizes discrete events occurring independently of one another in time. It is frequently used to model random and time homogeneous earthquakes.⁷ For a discrete time step model such as the β -SOAR, the probability of n events occurring in a time step can be represented as

$$P(n) = \frac{(\lambda \Delta t)^n e^{-\lambda \Delta t}}{n!} \quad (1)$$

where λ is the mean event frequency (1/yr) of the Poisson process and Δt is the time step size (yr). For each time step, the cumulative distribution function (CDF) of the Poisson process needs to be calculated given a particular time step size Δt . The number of events that may occur during a time step could be subsequently obtained randomly from the CDF and uniformly distributed within the time period.

For each time step of the β -SOAR model, zero or multiple seismic events may be generated. Given a pre-determined, site-specific seismic hazard curve and a sampled event frequency from a given, site-specific, event frequency probability density function, an associated peak ground velocity of a seismic event can be determined from the seismic hazard curve. We note that, in the prototype discrete event model and for all the test cases used in this paper, the site specific data used are for model testing and demonstration purposes only.

II.B. Backfill and Impact on Waste Package

Depending on the design and geologic environment, a disposal system may reside in hydrogeologically

saturated or unsaturated zones. It may or may not have natural or engineered backfill materials surrounding waste packages. These considerations need to be accounted for in calculating potential damage to waste packages by disruptive events. Additionally, if backfill materials are used, they may degrade over the designed life time of the disposal system. In a repository located inside the unsaturated zone without backfill, the waste packages may move freely or partially freely, increasing the likelihood of waste package damage. For repositories inside the saturated zone, groundwater may fill in the space vacated from degraded backfill materials. To date, there is not controlled, precise characterization on the degree to which groundwater, in comparison with air, may reduce the mobility of waste packages once the backfill material has begun to degrade and disperse in a groundwater saturated environment. For the model conceptualization of this paper, we conservatively assume that groundwater does not reduce the mobility of waste packages, in comparison with air, if backfill materials are absent or have degraded to a certain level of their original state. We acknowledge the existence of uncertainty in model parameters and model results under this assumption.

For an individual waste package and disruptive event, damage may or may not occur, depending on the magnitude of the event and the remaining strength of the waste package material. To date, limited information is available in this regard. In particular, the waste package damage area caused by seismic ground motion has not been characterized or estimated for waste package materials such as copper, titanium, stainless or carbon steel, which are potential candidate materials for a variety of geological disposal systems.

Considering the impact of seismicity on individual waste package and uncertainties of the impact area, angle and location of impact, new relative to existing damage areas, existing crack density and remaining thickness of the waste package, new seismic event may or may not produce additional through wall cracks. While estimates are available for certain waste package materials, e.g., Alloy 22 and, to some extent, titanium⁸, data for other waste package materials are limited. Analysis of experimental results, however, suggests that crack area density, or crack area per unit damage area resulting from seismicity, could be expressed as a function of waste package material yield stress (σ in MPa) and Young's modulus (E in MPa) for stress corrosion cracking (SCC) as follows⁸:

$$\delta = C \frac{\sigma}{E} \quad (2)$$

where δ is the crack area density (m^2/m^2) and C is a scaling or uncertainty factor accounting for crack network geometry. On the basis of equation (2) and industry data sources, e.g., Metals Handbook⁹ by ASM International, of yield stress and Young's modulus for the waste package materials of concern to this research, the crack area density can be estimated to, for example, range from 5.0×10^{-4} to 0.02 for copper and from 2.0×10^{-3} to 0.07 for titanium (Table I), by using uncertainty factors from 1 to 8 in equation (2). In this paper, the example case is chosen for SCC because SCC is generally dominant in waste package damage, compared with the purely mechanical damage (e.g., puncturation).

Damage to ductile metals such as copper and carbon steel could be assessed on the basis of SCC models for less ductile materials such as Alloy-22. This is so because ductile materials undergo a brittle, SCC process as a result of mechanical damage. With this understanding, we calculated crack area density using equation (2) for all candidate waste package materials available in β -SOAR. The ranges of crack area density ratios for Alloy-22, stainless and carbon steel are similar (Table I). The more ductile copper has a slightly wider range than the above-mentioned three materials. The higher upper bound of titanium reflects more grades of titanium alloy than commercial, pure titanium metal itself. The similarity of crack area density among Alloy-22, stainless and carbon steel does not necessarily suggest similar, seismic damage areas or SCC configurations on these waste package materials. However, for model testing purpose, this paper assumes that they are similar. For formal application of the seismic model, however, more thorough investigation in this regard, with and without backfill materials and under groundwater saturated conditions, would be planned for future activities.

Because β -SOAR uses the concept of representative waste packages, it is necessary to assume that the fraction of the total number of waste packages that could be damaged by a seismic event also correlates, or proportions, to the probability that a waste package may be damaged by the same event. It is further assumed that for a subsequent event, damage may not occur to those waste packages that have previously been damaged until all the waste packages have been damaged. We also fix the thickness of the waste package material in these simulations so that we could isolate the effects of mechanic damage. Figure 1 compare the effects of these assumptions to an ensemble of 10,000 waste packages in which waste package damage events are tracked for individual waste packages. Because Alloy-22 is the only waste package material that has been thoroughly characterized for mechanical damage during seismic events, waste package damage fraction and area

calculations here (Figures 1 and 2) use information in Refs. 5 and 8 for illustration purposes only.

Table I. Crack Area Density

Material	Lower Bound	Upper Bound
Stainless Steel	0.16%	1.17%
Copper	0.05%	2.08%
Carbon Steel	0.18%	0.91%
Titanium	0.15%	7.31%
Alloy 22	0.29%	1.17%

Comparison of ensemble average and representative fraction of waste packages damaged by seismicity in Figure 1 suggests that the representative approach could result in earlier waste package damage. For example, 1 out of the 10,000 waste packages is damaged earlier using the representative waste package concept when backfill is present. If waste packages are allowed to move freely, the waste package damage time is about the same for both conceptualizations. For the majority of the simulation time, the difference between the two conceptualizations is small considering the large uncertainty related to waste package emplacement method (e.g., borehole or tunnel), backfill degradation, waste package and geologic

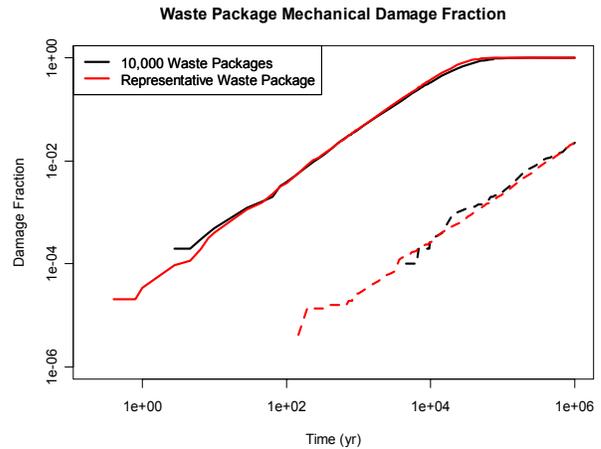


Fig. 1. History of mean fractions of waste package damaged mechanically in a repository with (dashed lines) and without (solid lines) backfill.

formation integrity, the impact of seismic ground motion on waste package damage, and waste package integrity. The comparison of waste package damage area from the two conceptualizations is shown in Figure 2, which also indicates small differences for damage areas larger than $1 \times 10^{-4} \text{ m}^2$. The results shown in the figures were obtained using the assumption that the backfill materials do not degrade over the lifetime of the disposal system. In reality, backfill materials could evolve over time. The difference in waste package damage fraction between the two repository designs, with and without backfill materials, should be smaller than that shown in Figure 1.

Nevertheless, the differences of the damage fractions and areas between disposal systems with and without backfill, around 2 to 3 orders of magnitude, suggest that characterization of backfill effects on waste package damage could further reduce model uncertainty.

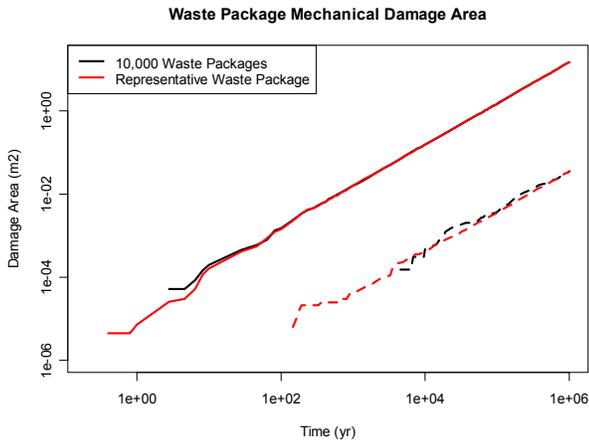


Fig. 2. History of mean waste package mechanically damage area in a repository with (dashed lines) and without (solid lines) backfill.

II.C. Conditional Discrete Events

Discrete events, e.g., conditioned on seismic events resulting in fault displacement and on early waste package failure, may damage all or a portion of the waste packages. These events could be modeled through the second or third level of flexibility built into β -SOAR. For level two flexibility, one may either directly change the onset time of localized corrosion in addition to specifying the fraction of waste package that may be damaged. This can be achieved by altering either the data contained in the respective elements in the model itself or those in the database that accompanies the model. In β -SOAR, localized corrosion is characterized by probability of waste package failure, which differs for individual, candidate waste package materials. For example, titanium waste package materials are assumed to be alloyed with noble metals such as palladium or ruthenium, which effectively prevents localized corrosion. For copper and carbon steel, β -SOAR models localized corrosion through a pitting enhancement factor to the general corrosion rates, because pitting corrosion of these materials is more widespread. For these materials, level three flexibility needs to be exercised. With this level of flexibility, users could add or change model elements of β -SOAR to control the timing, the percentage of waste package damaged during the event, and the breached area of the waste package.

III. MODEL IMPLEMENTATION

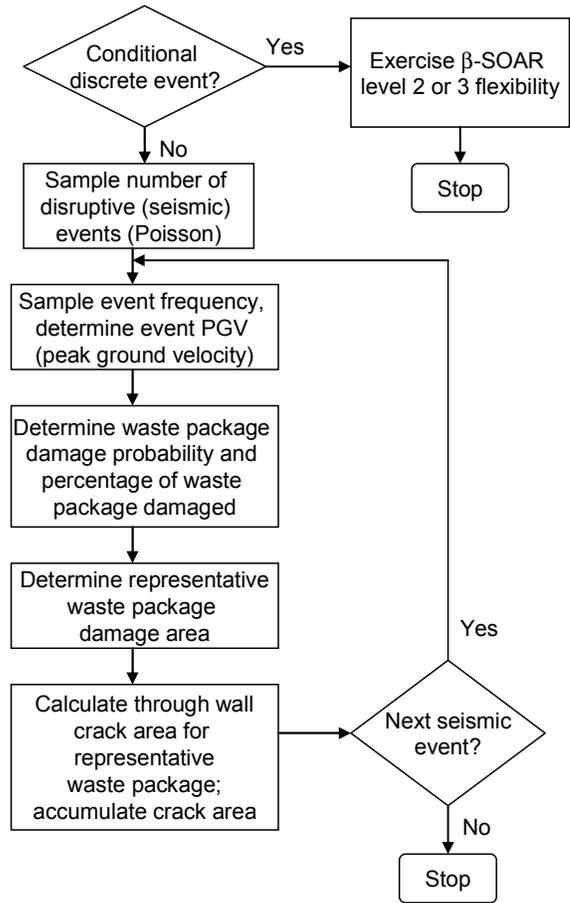


Fig. 3. Flowchart for a β -SOAR component model that calculates seismic and conditional discrete events and the subsequent waste package damage and failure.

The approaches described are implemented in a model branching off the main trunk of the β -SOAR code using the software GoldSim¹⁰. The flowchart above (Figure 3) depicts the modeling steps for the disruptive model prototype. Note that a conditional discrete event, e.g., seismic fault displacement, may not require model component modification (level 2 flexibility). For the purpose of this paper, a conditional discrete disruptive model is also implemented to demonstrate level 3 flexibility of the β -SOAR code.

The timed event element of GoldSim is used to generate a sequence of seismic events within a time step, which in turn trigger calculations of seismic peak ground velocity, waste package damage area and through wall crack area. The fraction of waste packages damaged by a seismic event, out of the total defined by users, is also calculated for the waste package component model of β -SOAR.

III.A. Integration with β -SOAR

Two approaches could be used to calculate waste package breach areas in β -SOAR: stepwise and average. The stepwise approach takes user inputs and increases the waste package breach area, from either general or localized corrosion, discretely at user specified times. The average approach calculates averaged breach areas weighted by the fractions of waste packages damaged by the two corrosion mechanisms. Detailed discussions on these two approaches are given in another paper in this conference¹¹. With seismic events, the through wall crack area is added directly to the total breach area when stepwise approach is selected. On the other hand, if average approach is selected, the fraction of waste package damaged by seismic events is used to add the weighted, seismic event breached area to that caused by the two corrosion mechanisms.

IV. TEST CASES

Two test cases were used to evaluate the disruptive event component model implementation. The geological formation is a groundwater saturated, fractured granitic rock in both near and far fields, including the immediate environments surrounding the waste packages. Matrix diffusion therefore may have additional impact to radionuclide transport in addition to adsorption. Because Alloy-22 is the only waste package material that has been thoroughly characterized for waste package mechanical damage during seismic events, waste package damage and failure calculations in these test cases use information in Refs. 5 and 8 for demonstration purposes only.

IV.A. Discrete Disruptive Event

The first test case is a discrete disruptive event that damages waste package materials, but not the waste forms, of all the waste packages in a disposal system. The discrete event occurs at the 10th year after the closure of the repository. It damages all waste package materials instantly. However, waste forms remain intact and the release of radionuclides into the near field is controlled by waste form dissolution and solubility of radionuclides (Figure 4). At the exit point of the far field (Figure 5), further reduction of release rates is caused by solubility of radionuclides in the near field and sorption and matrix diffusion in the far field under reducing conditions. The assumption that there is no backfill material also resulted in higher release rates of actinides such as Pu239 and Np237 in comparison with cases with backfill (results not shown). We note that, in β -SOAR, the default backfill material is bentonite with relatively high actinide sorption coefficients.

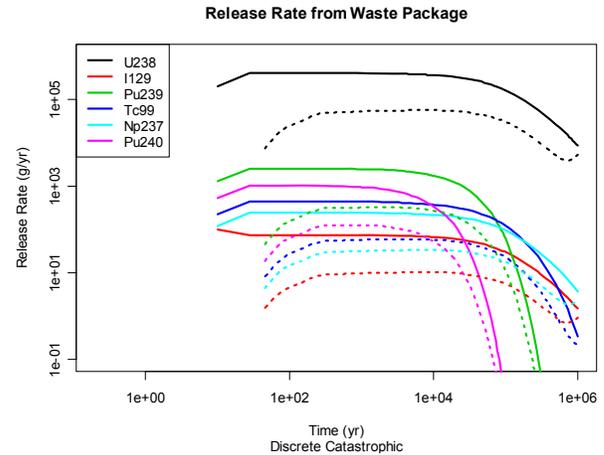


Fig. 4. Calculated release rates (solid lines) of U238, I129, Pu239, Pu240, Tc99 and Np237 away from the waste forms after the assumed discrete event damages all waste package materials at year 10. Dashed lines are the baseline case without the event.

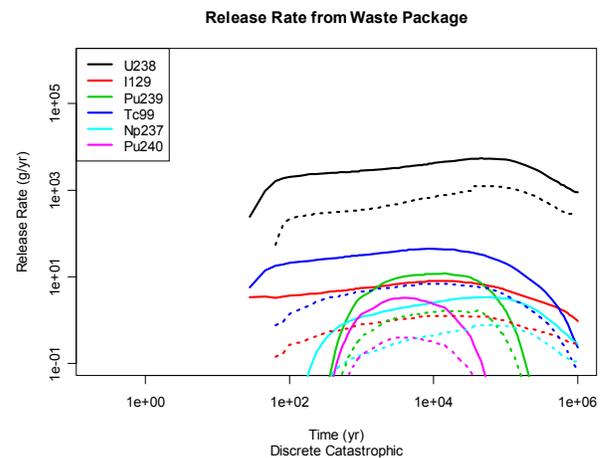


Fig. 5. Calculated release rates (solid lines) of U238, I129, Pu239, Pu240, Tc99 and Np237 at the far field exit point after a discrete event damages all waste package materials at year 10. Dashed lines are the baseline case without the event.

With the β -SOAR model, one performance measure of compliance is the integrated release. Figure 6 illustrates the integrated and individual radionuclide empirical, total release, complementary cumulative distribution functions (CCDF). Figure 6 suggests that the radionuclide release modes in a reducing environment could have an impact on the release. The discrete event moves the release curves toward higher exceedance probability (dashed to solid curves).

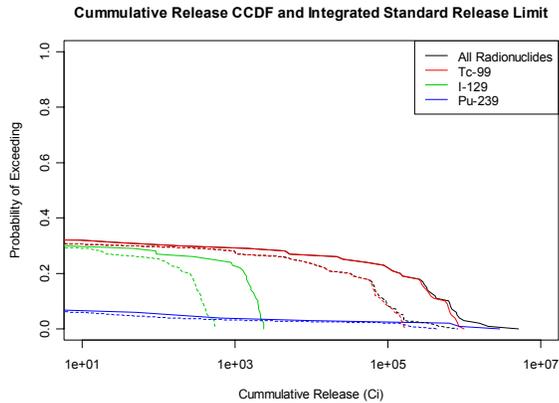


Fig. 6. Integrated release of selected radionuclides: Tc99, I129 and Pu239, for the discrete disruptive event (solid lines) and the baseline case (dashed lines).

IV.B. Seismic Ground Motion

The second test case is a geologic disposal system within a groundwater saturated, granitic geologic formation that experiences seismic ground motion under reducing conditions. A mean seismic event frequency of 4.3×10^{-4} 1/yr is used, and the hazard curve, waste package damage and failure characterizations in Refs. 5 and 8 are used, for demonstration purposes only. General corrosion rates varying between 0.1 and 10 $\mu\text{m}/\text{yr}$ and a mean waste package breach fraction of 0.05 (or 2 m^2) were selected for the simulation. These values represent a carbon steel waste package material. We note here that the range of crack area density values of carbon steel is similar to that of Alloy-22 (Table I). While this does not necessarily suggest that the crack area density equation (2) and its underlying assumptions, derived on experimental basis of Alloy-22 crack networks and crack sizes distribution, may be applicable for carbon steel, for model testing purpose, carbon steel was chosen as the waste package material for this simulation. The emplacement tunnel is not backfilled with natural or engineered buffer materials and waste packages could freely move in all directions in the tunnel in saturated groundwater. Because there are not experimental data or calculations available for waste package dynamic and mechanical damage under water, groundwater is assumed to have no dampening effects in reducing the seismic dynamic and mechanical damage on waste packages. It is essentially treated as air in this simulation.

Carbon steel, in general, is not susceptible to localized corrosion in reducing environments. As shown in Figure 7, before general corrosion fails the entire waste package at 10,000 years, breach area resulting from mechanical damage is the sole cause for waste package

failure. The breach area due to seismic ground motion, however, is more than three orders of magnitude smaller than general corrosion at the time immediately before general corrosion fails the entire waste package.

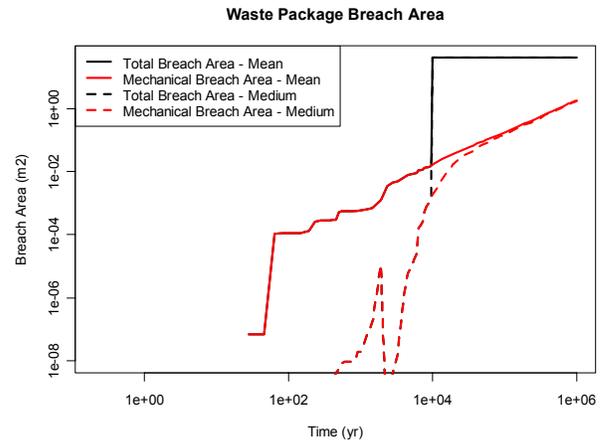


Fig. 7. Waste package breach areas: total from seismic mechanical damage, localized and general corrosion (black lines) and from seismic mechanical damage only (red lines).

With waste package failure caused by seismic ground motion, radionuclides could be released earlier from the near field and in a relatively larger amount compared to the baseline, nominal test case (Figure 8). For example, the peak release rate of Pu239 is calculated to be one order of magnitude higher and the time of peak release rate is about 3,500 years earlier. These results demonstrate the need to consider the contribution of seismic events to radionuclide releases from the near field in geological disposal systems that may be prone to earthquakes or tectonic activities.

At the exit point of the far field, Figure 9 illustrates the larger and earlier contributions to receptor doses by the seismic ground motion test case. For example, dose attributable to Pu239 is calculated to peak around 28,000 years for the seismic test case, compared to 68,000 years for the baseline, nominal test case. The peak dose rate of Pu239 calculated for the seismic test case is again one order of magnitude higher than that for the baseline test case (Figure 9). We note again that the high doses attributed to Pu and Np result from the assumption that there is not bentonite backfill material to reduce the release of actinides from the near field. The radionuclides are released directly from the waste package into the rocks surrounding the near field. A bentonite backfill material is also a diffusive barrier. It increases the residence time of water inside and surrounding the waste package, thereby allows more actinides in the precipitated phase as the waste and waste matrix dissolve. Without the

diffusive barrier and with a shorter residence time, a larger amount of Pu and Np could move into the far field and eventually increase the radionuclide doses at the far field exit point. Additionally, certain assumptions could be made with respect to radionuclide transport in the geosphere that can have significant effects on the timing and magnitude of radionuclide release to the biosphere. For example, there are a number of site specific attributes that may affect radionuclide transport in the geosphere. As of the writing of this paper, β -SOAR uses only attributes of a general nature.

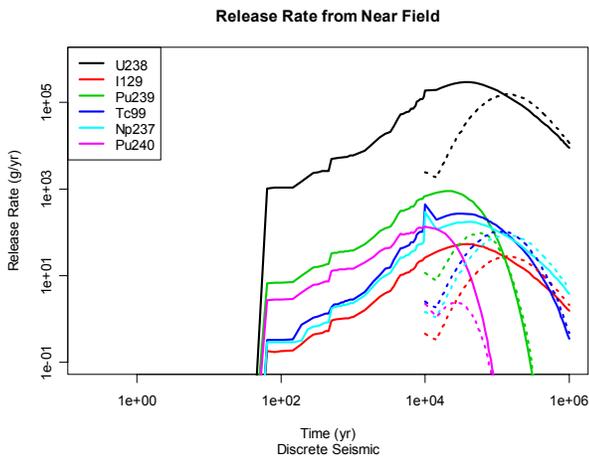


Fig. 8. Release rates of radionuclides away from the boundary of the near field into far field for the seismic ground motion test case (solid lines) and the baseline test case (dashed lines).

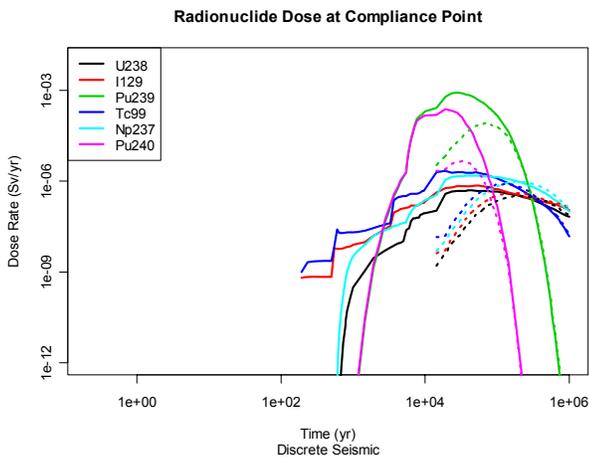


Fig. 9. Radionuclide dose curves at the compliance points for the seismic ground motion test case (solid lines) and the baseline scenario (dashed lines).

Because of the need to calculate waste package damage areas and crack area density ratios for the above seismic ground motion component model and also for the purpose of the β -SOAR model, it may be desirable to

simplify the model implementation. As of the writing of this paper, NRC staff is working on further abstracting the seismic ground motion component model, for the purpose of reducing data requirements.

V. DISCUSSION

The abstractions of disruptive events and their effects on waste package damage and failure inevitably introduce simplification from a process-level, mechanistic-based approach to a system-level, more abstractive approach. Additionally, there is a relatively long list of uncertainties regarding discrete disruptive event frequencies and magnitudes, locations within the geological disposal system that may be the sources or centers of disruptive events. Uncertainties also exist in the likelihood of waste package damage, the size of damage, and the ratios of damage to through wall crack areas.

The above results from the exercises of disruptive event component model implementation and integration with the β -SOAR model, nevertheless, suggest that, once a geologic disposal system is identified, the most likely insights regarding model uncertainty and geologic disposal system performance with respect to disruptive events could benefit from the following activities:

- Consideration of the effects of waste package emplacement method, e.g., borehole and tunnel, on waste package damage and failure from disruptive events;
- Consideration of integrity of backfill materials, and its evolution over the lifetime of the disposal system, including impact from seismic events and groundwater flow and transport;
- Consideration of the likelihood of waste package damage with various proposed backfill materials and when the backfill materials may be partially damaged;
- Consideration of waste package integrity as impacted by general and localized corrosion, which could in turn affect the strength of waste packages to withstand seismic impacts;
- Consideration of waste package damage area and through wall crack network geometry for the various types, designs and configurations of waste packages.
- Consideration of quantitative seismic-induced SCC model including the damage and crack areas.

VI. CONCLUSIONS

This paper describes the implementation and integration of a disruptive event and consequence model prototype with the β -SOAR code. We also present results

from two test cases, a discrete waste package damage bounding event and a seismic ground motion event that cause total and incremental waste package damage and failure, respectively. While the calculations and their results are for demonstration purposes only, they point to topical areas for further consideration to enhance the quantification of uncertainties and to fulfill data requirements of the β -SOAR model. These topical areas include the effect of backfill materials and their degradation on waste package damage and failure as resulted from seismic events and the likelihood of waste package damage, waste package damage area and through wall crack networks produced by seismic events. For the latter, needs are particularly noticeable for waste package materials other than Alloy-22.

ACKNOWLEDGMENTS

The authors wish to thank colleagues at NRC and CNWRA for assisting in developing and integrating the disruptive event component model and for reviewing this paper. In particular, we are in debt to Dr. Osvaldo Pensado for his generous input in integrating the seismic event consequence component with the waste package damage component of the β -SOAR model. The NRC staff views expressed herein are preliminary and do not constitute a final judgment or determination of the matters addressed or of the acceptability of any licensing action that may be under consideration by the NRC. This paper is also an independent product of the CNWRA® and does not necessarily reflect the view or regulatory position of the NRC.

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