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Use of Virtual Tracers in Repository Performance Assessment Modeling

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A primary objective of repository modeling is identification and assessment of features and processes providing safety performance. Sensitivity analyses typically provide information on how input parameters affect performance, not features and processes. To quantify the effects of features and processes, tracers can be introduced virtually in model simulations and tracked in informative ways. This paper describes five ways virtual tracers can be used to directly measure the relative importance of several features, processes, and combinations of features and processes in repository performance assessment modeling.

INTRODUCTION

A sensitivity analysis is known to provide useful information on how model inputs affect repository simulation performance metrics.[1,2] Sensitivity analysis methods include scatterplots, correlation coefficients, and variance-based decomposition indices which measure the fraction of an output variance attributable to each input parameter. However, a sensitivity analysis generally does not measure the degree to which performance is affected by features and processes. Quantification of performance sensitivity to these larger factors can be especially useful in the early phases of a repository program because it can help with siting and design decisions. For example, if it can be shown that dispersion alone prevents receptor dose rates from exceeding safety limits, then a high degree of performance may not be needed from the waste package outer barrier. For another example, if instant release fractions dominate the dose rate, then complex waste form degradation models may not be needed.

To quantify the effects of features and processes on performance, tracers can be introduced virtually in model simulations and tracked in informative ways. Virtual tracers can be introduced as a spike in the repository at the beginning of the simulation, as a constant injection in the repository over time, as fully released from a waste package upon waste package breach (i.e., not limited by slow waste form degradation), and as reactive tracers (e.g., decaying, adsorbing). Depending on how they are introduced and their properties, virtual tracers can be used to answer questions like:

1. How well does the repository region retain a tracer in its pore space?
2. What is the mean travel time of a tracer from the repository to the receptor?
3. How much does dispersion attenuate radionuclide concentrations?
4. How much do specific radionuclide release mechanisms and sources affect receptor dose rates?
5. How much does waste form performance reduce receptor dose rates?

Sensitivity analyses can, in turn, be performed on virtual tracer results to determine how model inputs affect tracer measurements. To date, in crystalline repository reference case simulations using PFLOTRAN, Dakota, and GDSA Framework (pa.sandia.gov), virtual tracers have been designed (but not fully tested) to address each of the five questions above. This paper summarizes and discusses the plans and results to date.

METHODS

Hydrologic Retention in the Repository

1. How well does the repository region retain a tracer in its pore space?

For a simulation of a water-saturated repository, this tracer measurement captures the combined effects of advection and diffusion on the transfer of released radionuclides beyond the repository and into the host rock. Advection is controlled by water flow through the repository. Diffusion is controlled by porosity and tortuosity within and around the repository. A spike of an aqueous conservative tracer in the repository region at the beginning of the simulation can be used to directly measure repository hydrologic retention owing to the combination of advection and diffusion in the repository region.

Fig. 1 shows the mass of initial tracer retained in the repository region over time for 20 discrete fracture network (DFN) realizations of a crystalline repository reference case.[3,4] These results indicate that the hydrologic properties of the repository alone provide significant waste isolation performance. The median residence time of the tracer in this figure ranges from about 50,000 to 130,000 years. Median residence time measurements are particularly intuitive and useful in sensitivity analyses. They can be used to identify factors that affect hydrologic retention in the repository (e.g., buffer porosity) and how important hydrologic retention is to overall repository performance.

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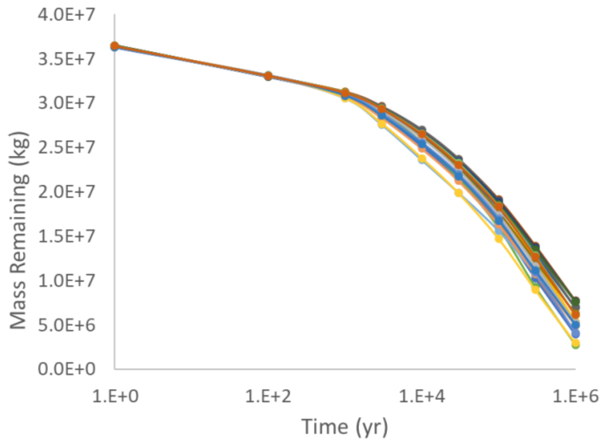

Fig. 1. Mass of initial tracer spike remaining in a crystalline repository reference case over time for 20 realizations.[4]

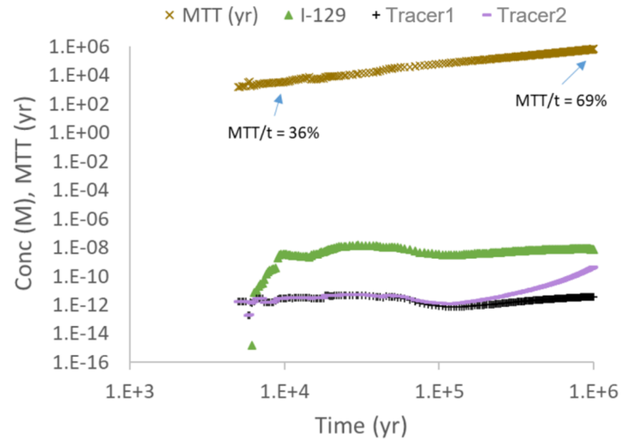

Fig. 2. Mean travel time (MTT) to receptor location, calculated from a simulation providing virtual tracer concentrations at the receptor.[4]

Mean Travel Time

2. What is the mean travel time of a tracer from the repository to the receptor?

The mean travel time (MTT) measurement uses two tracers, one of which decays or ingrows exponentially. If these two tracers are injected at the same rate over time into the repository, the mean travel time to a distant location can be calculated from:

$$\mathrm{MTT} = \frac{-\ln\left({C_2}/{C_1}\right)}{\left({\ln 2}/{t'}\right)} \qquad (1)$$

where C_1 and C_2 are the concentrations of the conservative and decaying/ingrowing tracers (Tracer1 and Tracer2) at the distant location and t' is the half-life (or doubling time) of the decaying (or ingrowing) tracer.[4]

Fig. 2 shows the MTT calculation and the concentrations of Tracer1, Tracer2 (ingrowing), and ^{129}I at the receptor for one realization of the crystalline reference case referenced in the previous section. As shown, MTT increases with time in this application. At t = 10,000 years, MTT is approximately 3,600 years (MTT/t = 36%). At one million years it is around 690,000 years (MTT/t = 69%).[4] The very high MTT calculation at one million years indicates that slow pathways are large contributors to the tracer concentrations at the receptor at that time. Differences in MTT between DFN realizations can potentially help explain why certain realizations have higher peak ^{129}I concentrations at the receptor location.

Dispersion

3. How much does dispersion attenuate radionuclide concentrations?

Solute concentrations in a plume attenuate downgradient due to dispersion, decay, and non-steady-state conditions (e.g., slow diffusive exchange into and out of dead-end voids). Dispersion of a solute occurs due to mixing of the medium (water) and diffusion within the medium. Mixing is caused by the branching and merging of flow as a result of pore space tortuosity, intersecting fractures, and heterogeneous flow systems. Fig. 3 shows modeled effects of dispersion due to fracture-dominated transport from a hypothetical repository in crystalline rock to an overlying aquifer.

A direct way to measure overall dispersion between a source and a receptor location in a simulation is to set a constant tracer concentration at the source and run the system to steady state. At steady state, the ratio of the tracer concentration at the source to that at the receptor provides an effective dispersion factor that quantifies the overall attenuating effect of dispersion in the simulation.

Repository reference cases, clearly, are not steady state simulations. The initially high and decaying thermal output of the waste packages over time cause transient changes to the flow field, as do other processes and events that may be modeled (e.g., corrosion, buffer evolution, earthquakes, glaciation, etc.). Nevertheless, measuring a dispersion factor at the end of a simulation period, e.g., at one million years, is expected to provide 1) an indicator of the magnitude of the effects of dispersion between the source and the receptor and 2) another way to characterize bulk system properties of individual stochastic realizations of spatial heterogeneity (e.g., different randomly-generated discrete fracture networks) so that the effects of dispersion and its uncertainty on repository performance can be better understood. This tracer measurement has not yet been demonstrated, but it is in the planning.

Fig. 3. Overhead view of dispersion of ^{129}I concentrations in a simulation of a homogeneous shallow aquifer above a hypothetical repository in crystalline rock. The rectangle shows the extent and location of the repository 560 meters below the aquifer. Warmer colors show higher ^{129}I concentrations.

Radionuclide Release Mechanisms and Sources

4. How much do specific radionuclide release mechanisms and sources affect receptor dose rates?

The concentration of a radionuclide at a downgradient location, as calculated using a performance assessment model, does not provide a breakdown of the relative contributions of different sources or source mechanisms. This is unfortunate because it would be useful to know how much of the resulting concentration originated from a specific source or mechanism (e.g., instantly released upon waste package breach, congruently released via slow degradation of the waste form, generated by ingrowth, released from a specific type of waste form or waste package, etc.). This information would directly measure the relative effects of the various sources and mechanisms on receptor dose.

Some of this information can be obtained from careful sensitivity analysis. However, much can be lost in the noise. If, for example, uncertainties in other aspects (e.g., waste package degradation rates or discrete fracture networks) dominate the uncertainty in radionuclide concentrations at the receptor, then the effects of different sources or source mechanisms are difficult to discern with a high degree of confidence. With the use of tracers, however, the contributions of the various sources and mechanisms can be determined precisely and without subsequent sensitivity analysis.

Separate tracers can be defined to represent instant release fractions, fuel matrix degradation fractions, fuel type fractions, waste package type fractions, etc. Fig. 4 illustrates how tracers would be assigned for a radionuclide released from two different waste packages (or waste forms) by two different mechanisms. As needed, the tracers can be given the properties of the major radionuclides that contribute to dose at the receptor (e.g., radioactive decay half-lives, adsorption properties, diffusion properties). If ^{129}I is the major contributor to dose, then each tracer for this measurement must also have the same properties and distribution among the sources and source mechanisms so that the total concentration of this tracer at the receptor will be the same as the ^{129}I concentration from the same sources. That way, the relative concentrations of the tracers at the receptor will indicate the relative amounts from each source and source mechanism.

Simulations using different tracers for the instant release fraction and the fuel matrix degradation fraction are underway. Further breakdown of tracers by package type is proposed for subsequent studies.

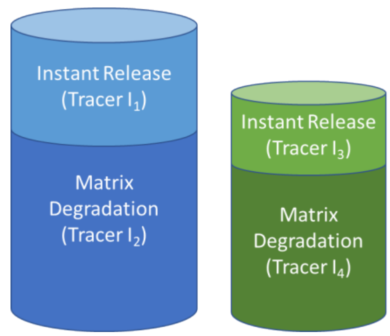

Fig. 4. To track the source and release mechanism of a specific radionuclide for two waste sources and two release mechanisms per source, four tracers would be needed.

Waste Form Performance

5. How much does waste form performance reduce receptor dose rates?

Does waste form performance cut receptor dose rates by a factor of 10, 100, or more? How does it affect releases to the biosphere over time (e.g., Fig. 5).

Without virtual tracers, these questions could be answered by running separate simulations: one including the nominal waste forms and one releasing the waste form inventory as soon as the waste package breaches. With tracers, this question can be answered in a single simulation: simply include tracers in the waste form that have the same properties as the important radionuclides except that they have 100% instant release fractions. As long as these tracers are set up to mimic the behavior of the important radionuclides throughout the system, dividing the peak "dose" rates of these tracers at the receptor by the peak radionuclide dose rates will directly provide the dose reduction factors attributed to waste form performance.

Adding tracers to the simulations adds to the computational time. However, much more computational time would be required to run separate simulations, one including waste form performance and one without. Exactly how much computational time reduction may be realized will be determined as we test this tracer measurement in future studies.

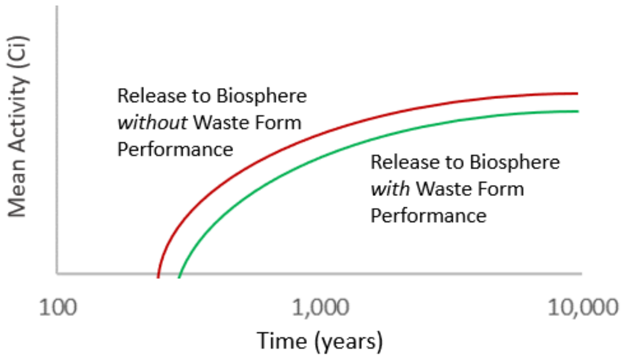

Fig. 5. Hypothetical comparison of releases to biosphere including (green) and excluding (red) waste form performance.

CONCLUSIONS

Five numerical tracer applications are described in this paper that are useful in studying repository system model behavior and the effects of specific components in the model. The first three applications provide ways to measure specific bulk effects of the hydrologic system in a simulation (repository retention of a tracer, mean travel time to a receptor, and overall dispersion). The fourth application provides a way to directly quantify the contributions of different source types and source release mechanisms on the receptor dose rate in the simulation. The fifth provides a way to directly quantify the performance provided by a slowly degrading waste form.

Adding virtual tracers to a repository system model will not affect radionuclide behavior in the model. A drawback is that it will increase computational time, but likely not prohibitively. Regardless, because the information provided by virtual tracers is highly useful in measuring bulk effects and clarifying the effects of various components and processes in a simulation, it may become routine to use virtual tracers in repository performance assessment simulations and subsequent sensitivity analyses.

ACKNOWLEDGMENTS

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