MULTIPLE SPECIES AND INGROWTH MODEL IN FEHM

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I. INTRODUCTION

The Finite Element Heat and Mass transfer code (FEHM, Zyvoloski, et al., 1995) developed at Los Alamos National Laboratory has been used in the performance assessment analyses to study flow, heat, and radionuclide transport at the potential high level nuclear waste repository site at Yucca Mountain. To better serve the need of the performance assessment analyses on radionuclide transport in the geological media, we expanded the single species particle tracking module to include multiple species radionuclide decay and ingrowth. With the new FEHM particle tracking module, we can simultaneously simulate the transport process of heavy radionuclides with multiple decay chains.

II. METHODOLOGY

The extension of the particle tracking module from single species into multiple species was straight forward. To improve the efficiency of simulations, we modified the original program to calculate the flux, fracture-matrix flow interaction, and retardation factors before the call of the particle tracking module. By doing this, we increased the efficiency of simulations by about 20%.

For the decay-ingrowth simulation with time dependent release of tracer particles, the computational burden increases dramatically with the number of particles in the field. For example, the decay-ingrowth calculation for species i with a decay rate λ decays into species j is:

$$N_j = \sum_{m=1}^{N_i} \{1 - \exp[-\lambda(t - t_m)]\} \quad (1)$$

where N_j is the number of particles of species j decayed from species i , N_i is the number of particles of species i , and t_m is the time at which the m th particle is injected into the system. If we inject 500,000 particles of species i into the system, then at each time step, the number of mathematical operations for ingrowth calculations alone are around 2.5 million. To simulate a time period of 1 million years, the typical calculation requires about 200 time steps. Therefore, the total number of operations for ingrowth calculations will reach 0.5 billion. It is obvious, for site scale sensitivity study, the use of equation (1) inside FEHM is inefficient.

To reduce the computational burden in simulations, we approximate the decay-ingrowth calculation in equation (1) with an integral. Multiplying both sides of equation (1) by dt , the average injection time interval between particles, we have:

$$N_j = \left\{ (\tau_2 - \tau_1) + \frac{1}{\lambda} \cdot [\exp(-\lambda\tau_2) - \exp(-\lambda\tau_1)] \right\} / dt \quad (2)$$

where $\tau_1 = t - t_1$ and $\tau_2 = t - t_{N_i}$. Using equation (2), we are able to reduce the amount of operations within one time step from millions of operations to just 10, which greatly increases the speed of simulations.

The accuracy of the integral approach depends on the number of particles and their release history. In general, the use of more particles increases the accuracy. When the same number of particles is used in simulations, the one with the constant release rate has less error. If the release rate changes with time, we divide the release period into several segments so that within each segment the release rate can be treated as constant. Then, the decay-ingrowth calculations are carried out corresponding to each segment.

We tested the integral approach against the discrete formula in equation (1). In most of our simulation runs, we released at least 100,000 particles for each species over the repository area (represented by 100 nodes) at a constant rate. The releasing period varied from 1,000 to 10,000 years. Test results from calculations at different times showed that in general, the results from the integral approach were very close to those from equation (1). The relative error was less than 1%. But, the computational burden was greatly reduced from millions of operations to just 10 operations within each time step.

Another issue that relates to ingrowth simulations is the distribution of the new species. In FEHM, we approach this problem by the rule of first in and first out. In the case where several particles are injected at the same time, a uniform random number generator is used to randomly pick up the decayed particle(s). The new particle(s) generated due to decay-ingrowth takes over the location of the old particle(s) but with its/their own transport properties.

III. CODE VERIFICATION

The multiple species ingrowth particle tracking model was tested against the Repository Integration Program (RIP, QA version 5.16, Golder, 1997) using a 1 meter long 1-D saturated field with pseudo radionuclides. A constant flow field was established so that the travel time for conservative tracers was 3,900 years. A total of 7 species with the same transport properties were simulated. A multiple decay chain starting from species 1 then sequentially decayed into species 6 (1->2->3->4->5->6) was assumed in the simulations. The half lives of species 1 to species 5 were: 10, 100, 1,000, 10,000, and 100,000 years, respectively. We injected 500,000 particles of species 1 (representing 100 gram radionuclides) into the system at a constant rate from 0 to 5,000 years. Species 2 to species 6 had initial concentrations of zero. Species 7 which had the same release history as species 1 but without decay was used for comparison. Since RIP directly solved the radionuclide transport equations, a dispersivity of 0.025 m was used in RIP and FEHM simulations to reduce the effect of numerical dispersion in RIP.

The mass flow rate curves at the outflow boundary from FEHM and RIP simulations are plotted in Figure 1. Due to numerical dispersion, the RIP curves have longer tails than the FEHM curves. The mass flow rates of species 1 and 2 at the outflow boundary are extremely low because of their short half lives, 10 and 100 years, respectively, and the relative long travel time (3,900 years). In fact, species 1 was not observed at the outflow boundary during the simulations. On the other hand, the long half life of species 5 (100,000 years) and the relative short travel time (3,900 years) resulted in very little decay of species 5. Thus, the

mass flow rate of species 6 is also very low. It is clear that the FEHM curves match the RIP curves very well. The normalized cumulative curves from the FEHM simulation are plotted in Figure 2. At any given time, the summation of fraction values of species 1 through species 6 equals the fraction value of species 7, which indicates the conservation of mass in the system.

Figure 1. Comparison of mass flow rate curves from RIP and FEHM. The mass flow rates of species 1, 2, and 6 are too low to be seen in this figure.

Figure 2. Normalized cumulative breakthrough curves from FEHM. The normalized values for species 1, 2, and 6 are too low to be seen in this figure.

IV. CONCLUSIONS

The FEHM multiple species decay-ingrowth particle tracking model was developed and tested. The initial test results showed that the code was able to correctly simulate the radionuclide transport and ingrowth process. With the new FEHM particle tracking module, we can simultaneously simulate the transport process of heavy radionuclides with multiple decay chains and better serve the needs of system performance assessment.

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