SAND2007-0171P

Supplemental Information on Models and Software Used for Fate and Transport Modeling of the Mixed Waste Landfill

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December 7, 2006

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

1. Tritium Transport Model

The fate and transport of tritium was simulated using a model that accounts for transient liquid advection, gas diffusion, and decay (Jury et al., 1983; Jury et al., 1990). The upper boundary condition at the surface allowed for gas-phase transport of tritium to the atmosphere across a prescribed boundary-layer thickness. The concentration at the bottom of the model was specified as zero infinitely far away from the source.

The implementation of the analytical model as described in Jury et al. (1983) and Jury et al. (1990) in this study can be checked by evaluating the Mathcad model, which is written in ordinary symbolic math. A PDF file of the Mathcad model is attached in the following link:

- Mathcad - Trititum_MWL_Jury et .pdf

In addition, a mass balance was performed on one of the realizations by comparing the total amount of tritium initially in the inventory to the total amount of tritium transported away from the system (via volatilization to the surface and liquid advection and gas diffusion downward to the water table). For this mass balance, the decay of tritium was assumed in the model to be zero. Also, because the transport is transient, the flux of tritium in each of the pathways was integrated over time. Figure 2 shows the transient plots of tritium mass flow through each of the pathways for one realization. Integration of these plots shows that the majority of tritium is lost via surface volatilization (2.02×10^{-4} kg), followed by aqueous advection (2.5×10^{-6} kg) and downward gas flow (2.8×10^{-7} kg). The cumulative mass lost is estimated from these plots to be 2.1×10^{-4} kg. For this realization, the initial inventory of tritium was 2.6×10^{-4} kg. Although not exact, the mass balance is reasonable given that the mass fluxes had to be integrated over thousands of years, and the resolution of the time steps was coarse (100 years in some cases). In addition, the transient plots shown in Figure 2 are physically sensible with regard to gas and liquid transport of tritium both to the surface and to the water table.

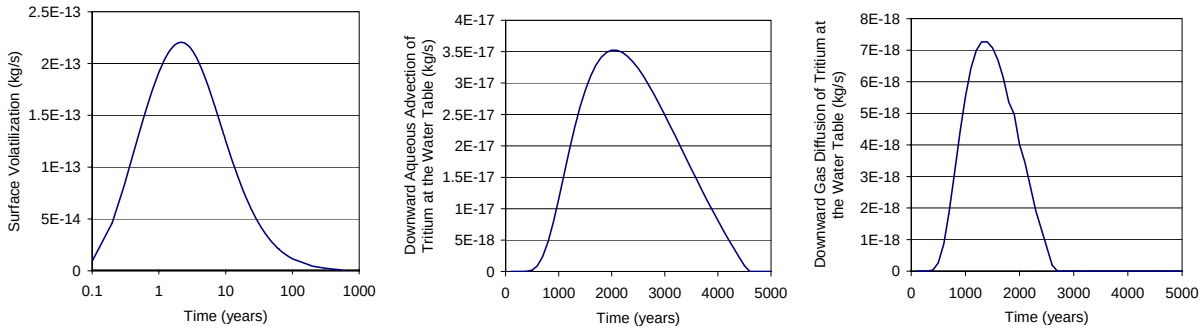

Figure 1. Plots of tritium loss from the unsaturated zone via three pathways assuming no decay. Left: surface volatilization. Middle: aqueous advection at the water table. Right: downward gas flux at the water table.

All of the inputs and outputs from the tritium transport model for all 100 realizations are included in an Excel file:

- Tritium_realizations.xls

2. Radon Transport Model

The radon transport model is described in Section **Error! Reference source not found.** and derived in Appendix A of Ho et al. (2005). The steady-state radon transport model that was developed for this study includes multi-phase diffusion, liquid advection, and decay of radon. A constant generation of radon is assumed to occur in the prescribed waste zone with a fixed source of radium.

The proper implementation of the model in Mathcad was verified by performing a mass balance on the amount of radon generated in the source zone versus the amount of radon leaving the system via both diffusion (upward to the surface and downward to the water table) and liquid advection to the water table. For this mass-balance check, the decay of radon was assumed to be zero (the half-life was set to 10^{20} s). Figure 2 shows that for all 100 realizations, the amount of radon generated was equal to the total amount of radon that left the system. The amount of radon leaving the system was calculated from fluxes based on concentrations and gradients that were reported in Ho et al. (2005).

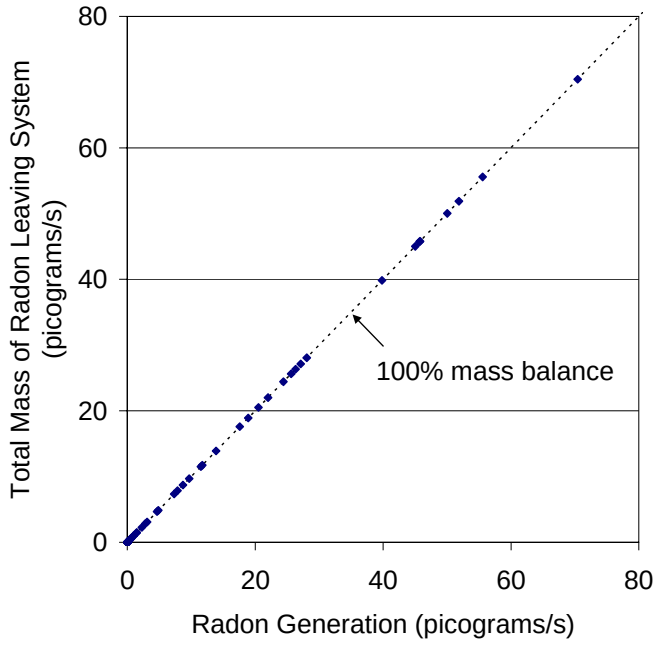

Figure 2. Plot of mass of radon leaving the system versus radon generated for 100 realizations assuming no decay.

A print-out of the radon-transport model in Mathcad is attached in the following file:

- Mathcad - Radon_transport_3-reg.pdf

Excel files containing the all of the inputs and outputs of the model that were presented in Ho et al. (2005) for 100 realizations are also attached:

- Radon_realizations_maxE_1.xls
- Radon_realizations_maxE_0.01.xls

3. Aqueous Radionuclide Transport Model

The aqueous radionuclide transport model (and the heavy-metal transport model described in Section 4) was developed using FRAMES v. 1.5 (Framework for Risk Analysis in Multimedia Environmental Systems; Whelan et al., 1997) and MEPAS v. 4.1.1. (Multimedia Environmental Pollutant Assessment System; Whelan et al., 1992). Software quality assurance has been maintained and reported by the developers of this software at Pacific Northwest National Laboratory (contact: Gariann Gelston, 509-372-6060, gariann.gelston@pnl.gov).

In addition to the validation and benchmarking performed by the developers, the specific modules used in this study (Source and Vadose Zone) were tested against analytical models. Figure 3 shows the problem definition for a test case that evaluates the leaching of radionuclides from a source zone in the vadose zone.

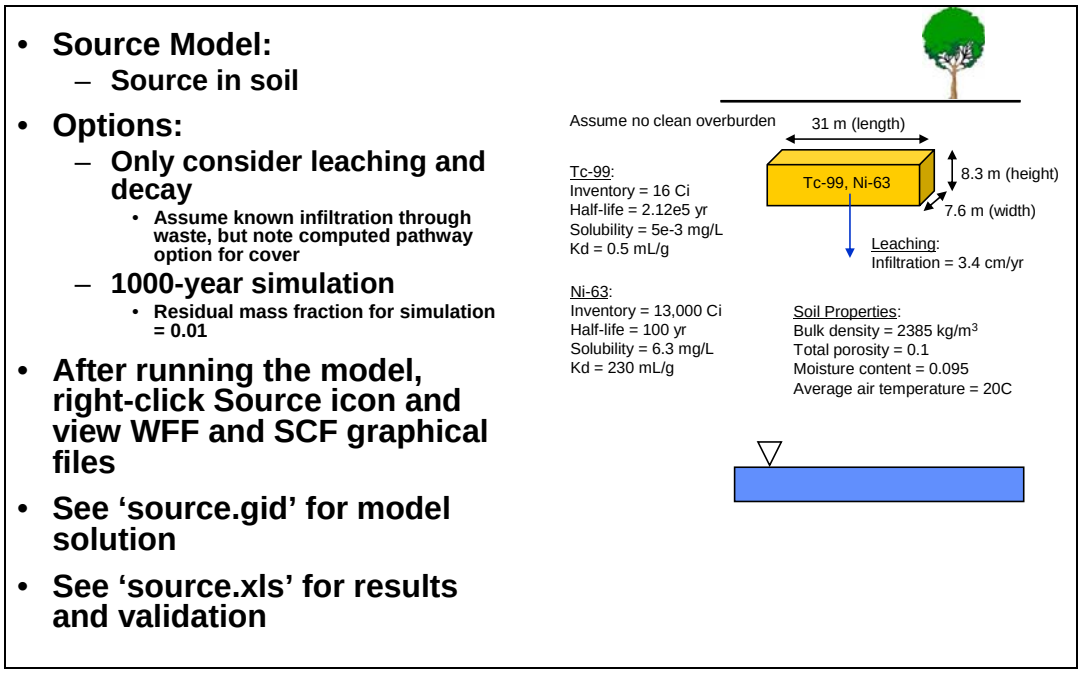

Figure 3. Test case of the Source module in FRAMES/MEPAS.

Results of the 1000-year leaching simulation for one of the radionuclides are shown in Figure 4. The analytical and FRAMES/MEPAS results are nearly identical, indicating that the code is performing as intended. The results of the test case and a description of the analytical method can be found in the attached Excel file:

- source.xls

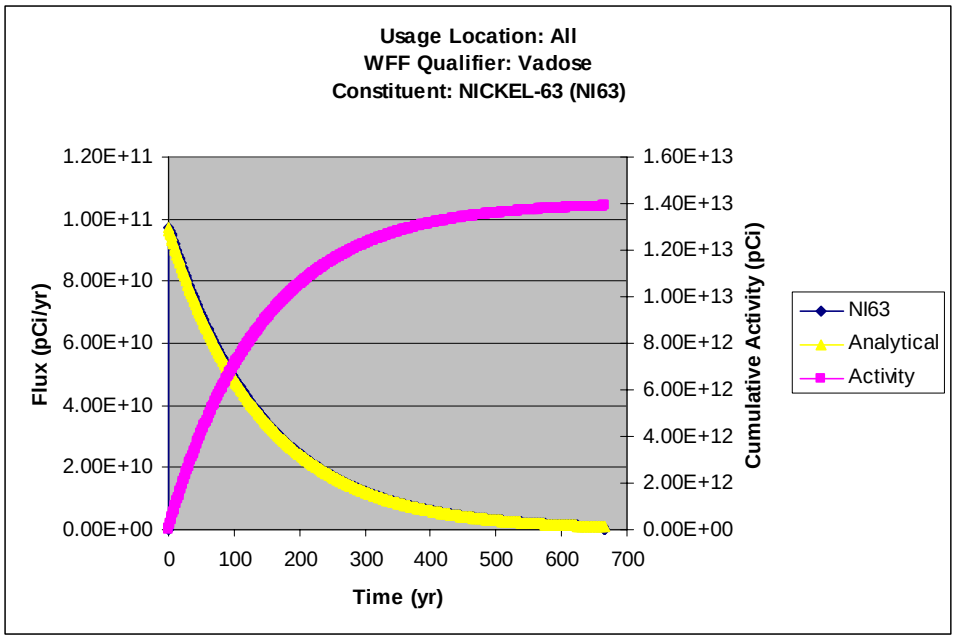

Figure 4. Comparison between FRAMES/MEPAS results and an analytical solution for the Source module.

Figure 5 shows the problem description for a test case that evaluates the transport of a radionuclide through the vadose zone. The concentration at the base of the vadose zone is calculated as the estimated contaminant flux (mass/time) divided by the water flux (volume/time). Figure 6 shows a comparison between the simulated and analytically determined concentration at the base of the vadose zone over a 1,000-year period. Results are nearly identical, indicating that the model is properly implemented within FRAME/MEPAS. Details of these results are included in the attached Excel file:

- vadose.xls

In addition to the documentation provided by Whelan et al. (1992, 1996, 1997) and Streile et al. (1996), a training presentation is attached that describes each of the modules in more detail than is presented here:

- FRAMES_Training.ppt

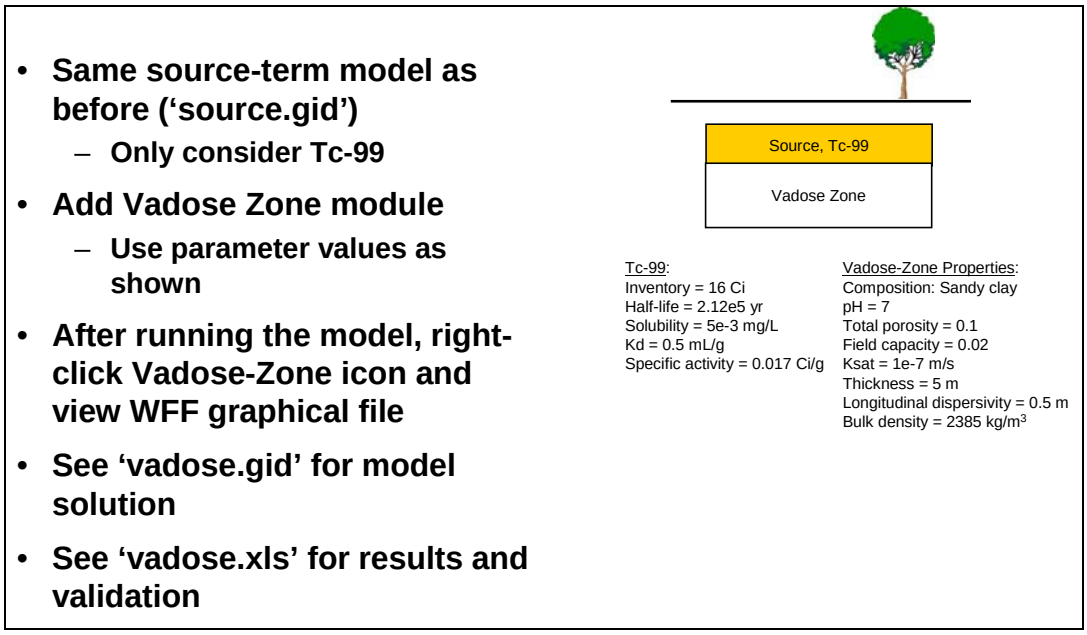

Figure 5. Test case of the Vadose Zone module in FRAMES/MEPAS.

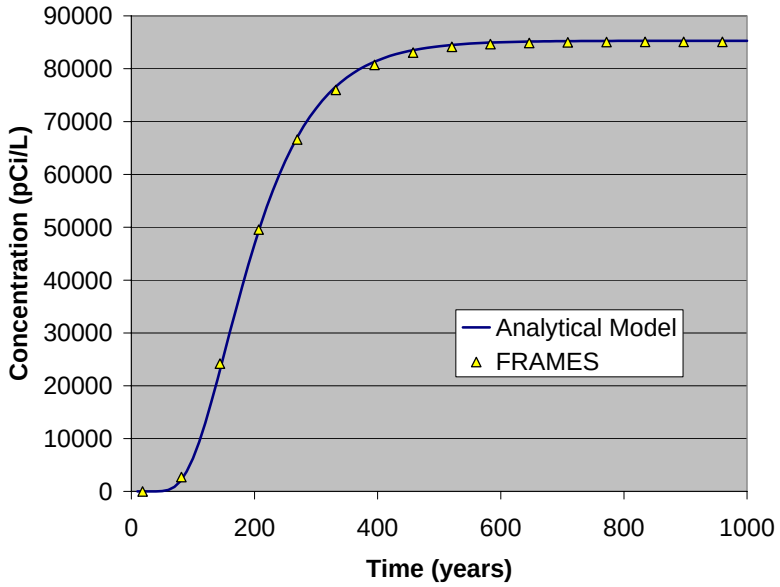

Figure 6. Comparison between FRAMES/MEPAS results and an analytical solution for the Vadose Zone module.

The FRAMES/MEPAS software was used to simulate the aqueous transport of radionuclides, as described in Section 3.7 of Ho et al. (2005). Additional details regarding the inputs and outputs for all 100 realizations and for each constituent can be found in the attached Excel file:

- allrads.xls

4. Heavy Metal Transport Model

The aqueous transport of lead and cadmium were also simulated using the FRAMES/MEPAS software, as discussed in Section 3.8 of Ho et al. (2005). The inputs and outputs for all 100 realizations are included in the attached Excel file:

- cadmium.xls
- lead.xls

Refer to Section 3 above for more details regarding the implementation of the Source and Vadose Zone models in FRAMES and MEPAS.

5. VOC Transport Model

The transport of PCE (as a conservative proxy for other VOCs) was simulated using the same model developed for tritium transport described in Section 1 of this supplement. The model was implemented in Mathcad and can be verified in the following PDF file:

- Mathcad - PCE_stochastic_variab.pdf

Section 3.9 of Ho et al. (2005) describes the PCE transport model and results. This supplement provides the inputs and outputs for all 100 realizations in the attached Excel file:

- PCE_realizations_souce-thickness10-27.xls

6. Summary

This supplement provided additional documentation regarding the models and software used in the fate and transport models presented in Ho et al. (2005). Mass balances and comparisons to analytical solutions were performed to verify that the models and software were implemented properly. The models and software can be summarized and grouped as follows:

- Transient analytical model of gas and aqueous transport with decay (Jury et al., 1983, 1990)
    - Tritium transport
    - PCE (VOC) transport
- Steady-state analytical model of gas and aqueous radon transport with decay (Ho et al., 2005, Appendix A)
    - Radon transport

- FRAMES v. 1.5 and MEPAS v. 4.1.1 (Whelan et al., 1992, 1996, 1997; Streile et al., 1996): advective and dispersive aqueous transport with decay and ingrowth
    - Radionuclide transport (Am-241, Cs-137, Co-60, Pu-238, Pu-239, Ra-226, Sr-90, Th-232, H3, and U-238)
    - Heavy metal transport (cadmium and lead)

References

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