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M E M O R A N D U M

DATE: February 12, 2001
TO: Mal Murphy [malmurphy@home.com]
CC: Danielle Fife **[**dfife@nrff.com]
RE: **SATURATED ZONE FLOW & TRANSPORT AMR Reviews**
Particle Tracking Model and Abstraction of Transport Processes
ANL-NBS-HS-000026

This AMR describes Particle Tracking methodology used in the UZ transport models. Key items include:

1. This AMR goes into considerable detail into the Particle Tracking methodology used in the UZ transport models. It also contains comparisons to analytical and numerical solutions. It relates primarily to the technology used, and not to specific analyses of YMP. Particle tracking is an extremely powerful method, but is not perfect. In Section 1, p. 11-12, the AMR states, "the accuracy of the method for dual-permeability flow systems was investigated in detail and found to perform best when the flow regime undergoes abrupt transitions at unit interfaces, and in cases for relatively low diffusion. Given these results, this AMR demonstrates that the particle-tracking model can be used in three-dimensional radionuclide transport simulations of the Yucca Mountain unsaturated zone *as long as the limits on the model are recognized and parameters are chosen accordingly*." [Italics added for emphasis.]

2. Some of the assumptions used in deriving the model are subject to interpretation, although in these cases the AMR states, "This assumption does not require verification." (Section 5.2, p. 16-17). Specifically,

a. "Fracture frequency, aperture and permeability are log-normally distributed." This is probably sufficiently accurate for permeability, but is a poor assumption for frequency, which is material and genesis dependent; and aperture, which is material, genesis and diagenesis dependent.

b. "The cubic law is a valid approximation for gas permeability in fractured rock at Yucca Mountain." This assumption is only true for perfectly flat parallel fractures, and is subject to variation for rough fracture faces. Even so, it probably doesn't matter.

c. "**Active fracture model appropriately accounts for reduced fracture/matrix interaction.**" You guessed it!

3. The model used basically decouples advective flow and diffusion/dispersion. This can have some problems, as they note in Section 6.1.2, p. 21, paragraph 2, that "Highly dispersive transport invalidates the assumptions of the RTTF particle-tracking technique." This would also be true of regions with low head gradient or slow flow.

4. **The incorporation of the active fracture model is the biggest problem with this AMR**. The γ fudge factor is described in Section 6.2.1, p. 30.

5. Sec. 6.2.2, p. 35, bottom paragraph. **"In the FEHM decay-ingrowth model, a first in, first out approach is used to select which particles undergo decay." This simplification, which reduces computational time, is flat wrong: radionuclide decay does not have a memory as to when a particle was injected into the particle tracker.** This assumption forces particles that were earlier injected to have a different decay mode than particles of the same isotope injected later. Depending on what's hot and what's not, this could lead to substantial underestimates or overestimates of breakthrough times.

6. Section 6.3, p. 45. Code verification is based on visual comparison to analytical solutions or results simulated with other programs. A "goodness of fit" test should be made to provide a numerical measure of the accuracy of the method.

7. Section 7, p. 78, paragraphs 2-3. **The possibility of grid orientation effects was noted, but not analyzed. If present, grid orientation effects could significantly underestimate or overestimate breakthrough times. Accordingly, the model should be rerun with grid orientation rotated 30°, 45° and 60° in the x-y plane, to evaluate the sensitivity to grid orientation**. Because of fractures being predominantly vertical, it is probably not possible to rotate the grid from the z-plane. The AMR makes the statement that "It may be that for these grids, orientation errors are small because the grid is aligned with the hydrostratigraphic units and thus are more likely to be aligned with the flow field. Thus, one of the RTTF particle-tracking technique's possible limitations should be minimized." This is not science, it is wishful thinking. To quote Ma Kettle from the film Ma and Pa Kettle at the Fair, "Mebby so. Then again, mebby not."