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CAVEATS, ASSUMPTIONS, CONSTRAINTS, LIMITATIONS

These data are intended for use in, or have been developed using specific numerical models. Numerical models can provide insight into the processes at work in subsurface flow and transport. However, numerical models are generated from a conceptual understanding of the flow and transport processes. This conceptual understanding relies on many assumptions. Furthermore, numerical model results are generally only applicable to the scale of the original model and the scale of the model's discretization. Major underlying assumptions of the numerical models used with these data include the following:

1. Darcian flow is assumed to provide an accurate description of the subsurface flow dynamics. Where flow is not laminar, the Klinkenberg effect is non-negligible, or other non-Darcian flow effects are non-negligible, this assumption may be violated.

2. The models used are assumed to accurately describe unsaturated flow processes. Generally van Genuchten's model for unsaturated flow is used, however, others may be used.

3. Local thermodynamic equilibrium for each grid element is an inherent assumption of the numerical models used with these data.

4. The ambient system and processes represented with these models are often assumed to be at steady-state.

5. Where the Richard's equation formulation is used (EOS9), gas is assumed to be a passive phase (i.e., flow of gas is not included in the calculations).

6. Where the EOS1G formulation is used, the liquid phase is assumed to be a passive phase.

7. When used, thermal calculations include heat transfer due to advection, conduction, and phase change processes.

8. When used, transport calculations include advection and Fickian diffusion processes.

Since the numerical model involves complex processes and complex geometry, there are implications to the assumptions listed above that are too difficult to be enumerated in the limited space available here. If you do not fully understand the implications of the general assumptions and caveats to the data outlined above, you should not use these data without first fully reading and comprehending the report that goes with these data and all the background material in the reference list of that report. In order to avoid misuse of these data, we strongly recommend that all users, regardless of their level of understanding, read the report that goes with these data.

If you need a copy of this report please contact,

Nuclear Waste Program
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1. Rock and fracture compositions are homogenous in space (within a given subdomain).
2. CO_2 is treated as an ideal gas and assumed at equilibrium with the aqueous phase.
3. The CO_2 pressure effect is assumed negligible on the liquid and vapor flow calculations (small CO_2 pressures only).
4. All aqueous species have the same diffusion coefficient in water.
5. For mineral solid solutions, end members are specified instead of true solid solutions.
6. The initial water composition in fractures is the same as in the matrix.
7. A specific, limited, set of reactant and possible product minerals is assumed to represent the chemical system.
8. Minerals follow the same reaction rate expression for precipitation as for dissolution.
9. No nucleation threshold is assumed for mineral precipitation .
10. Water produced by mineral reactions does not affect liquid saturations.
11. Mineral surface areas remain constant during a simulation.
12. The amount of precipitating/dissolving minerals does not affect the rock permeability.
13. The water density is constant (1 kg/l) and is not affected by salts (for chemical calculations only).

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