HLWYM NPEmails

From: Randall Fedors
Sent: Wednesday, October 17, 2007 7:42 AM
To: James Winterle; Jin-Ping Gwo
Cc: Jude Mcmurry; Scott Painter; Hakan Basagaoglu; John Bradbury; 'cmanepally@swri.edu'
Subject: Re: matrix diffusion workshop report section
Attachments: Matrix Diffusion Conceptual Model in TSPA__Gwo_16Oct07rwf.doc

Jack,
See attached for some comments that came to mind. The comment on the discrete fracture model terminology is one that we as a group need to reconcile.
--Randy

>>> Jin-Ping Gwo 10/16/2007 10:37 AM >>>
Jim,

Thanks. When I did the figure years ago, I had in mind the pressure gradient is from fracture to matrix. I'll modify that.

Regards,
Jack

>>> < jwinterle@cnwra.swri.edu > 10/16/2007 10:02 AM >>>
Jack,
I like what you wrote. It is a clear and succinct summary of the DOE approach. I notice in figure G-1, that the advection arrows both point in the same direction; I think they should the show both directions like the diffusive arrows do.

I am almost finished writing a summary of the DOE's EBS Transport Model with a similar level of detail. The EBS transport model also includes matrix diffusion and probably results in significant credit --perhaps as much or more attenuation of transport than in the UZ. So, it is definitely worth discussing in the report. Another feature of the EBS transport model is that it is implemented entirely in GoldSim and would be fairly easy to reproduce the model. I expect to have the summary finished this week.

--Jim

----- Original Message -----
From: Jin-Ping Gwo < jxg4@nrc.gov >
Date: Monday, October 15, 2007 4:02 pm
Subject: matrix diffusion workshop report section

> Jim,
>
> Attached please find a write-up of the alternative conceptual model
> section. Please feel free to edit.

>
> Jude,
>
> I veered from the TSPA-SR/FEIS because of dated information. The
> TSPA-SEIS model, if available soon, should give a better perview
> of the
> TSPA-LA model. As I can tell from the most recent FEHM model available
> to us, transfer functions indeed are one of the critical set of inputs
> for matrix diffusion calculations. If TSPA-LA uses the most recent
> FEHMcode, then their calculations in the particle tracking AMR should
> roughly correspond to their TSPA-LA results. I still cannot completely
> agree with the initial conditions they used for the conditional
> transferfunctions at grid-scale, but the overall impact to model
> uncertainty may
> be minor. I'll have to do a stand-alone FEHM calculation to
> determine if
> that's the case though.
>
> Regards,
>
> Jin-Ping (Jack) Gwo
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> U. S. Nuclear Regulatory Commission
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>

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Mail Envelope Properties (Randall.Fedors@nrc.gov20071017074158)

Subject: Re: matrix diffusion workshop report section
Sent Date: 10/17/2007 7:41:58 AM
Received Date: 10/17/2007 7:41:58 AM
From: Randall Fedors

Created By: Randall.Fedors@nrc.gov

Recipients:
"Jude Mcmurry" <jmcmurry@cnwra.swri.edu>
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Tracking Status: None

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MESSAGE	2506	10/17/2007 7:41:58 AM	
Matrix Diffusion Conceptual Model in TSPA__Gwo_16Oct07rwf.doc			182848

Options
Priority: Standard
Return Notification: No
Reply Requested: No
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1. We have to figure out a way to avoid concurring with DOE on their use of :discrete fracture model" to describe their heterogeneous realization that has preferential flow paths. I do not agree that modeling bulk flow on their grid scale qualifies as a discrete fracture model. I have been calling it a discrete feature model, but am open to suggestions. They are still representing flow in fractures (e.g., 1 mm aperture) using grids that are 0.5 m wide (or greater) in drift scale models of experiments. Remember, they get their flow field from the site scale model which has 100m grids at minimum. There conceptual model comparison is really a comparison of different realizations of grid cell property assignments.
2. To avoid being confusing, I think you avoid mentioning dual-porosity in the same breath as dual-permeability, especially since you are only talking about the UZ here. We can distinguish the dual-porosity conceptualization from the dual-permeability when the SZ discussion is brought in. A big reason to avoid mentioning dual-porosity here is that your discussion and Figure G-1 both clearly allude to a dual-permeability concept, which is the only conceptualization used for the UZ.
3. Consider adding a sentence on the active fracture model to provide a linkage to other parts of the report. The active fracture model restricts flow (only) from the fracture to the matrix, but not vice-versa. Is diffusion also restricted in the fracture-to-matrix direction by the area, but not in the matrix-to-fracture direction?

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Matrix Diffusion Conceptual Model in TSPA

The UZ transport model of TSPA uses a dual-permeability, dual-porosity conceptual model in which fluids and radionucildes can move through the UZ in either or both continua. Transfer of radionuclide mass between the two continua is modeled with two separate mass transfer mechanisms: (a) advective mass flux as a result of fluid

advection and (b) diffusive mass flux as a result of molecular diffusion across the fracture and matrix interface. The mass transfer mechanisms can be schematically illustrated as in Figure G-1:

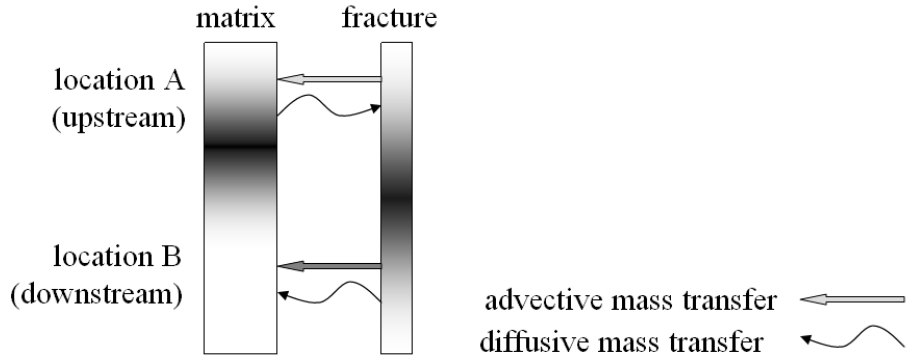


Figure G-1. Mass transfer mechanisms in a dual-permeability, dual-porosity UZ transport conceptual model.

In TSPA, the FEHM code is used to calculate UZ transport via a residence time transfer function (RTTF) particle tracking technique (BSC, 2004) through a three-dimensional network of connected cells (or nodes in numerical terms). The fluid mass flow rates between cells were pre-calculated by the computer code TOUGH2 and imported into FEHM for particle tracking calculations. Two sets of transfer functions were calculated in advance for FEHM input: (a) transfer functions for advection-dispersion within individual continua and (b) conditional transfer functions representing particle residence time probabilities within the continua in the presence of molecular diffusion but the absence of advective mass transfer across the fracture-matrix interface. The following discussion focuses on the latter part of the FEHM particle tracking calculations.

In FEHM calculations, once a particle enters a continuum, two more steps are required to determine its location and residence time in the next flow path segment. First, the

probability whether the particle should move to the other medium due to advective flux, or interflow, to that medium is determined. This step is equaled to '*a form of upwinding of the fracture-matrix fluid flux*' as suggested in BSC (2004) [clarify "form of upwinding" for the layman]. Second, the matrix diffusion portion of the fracture-matrix sub-model is represented by two sub-steps:

1. Use the steady-state or plateau of the conditional transfer functions in the fracture and matrix to determine the probability that a particle is to move to the other continuum. The conditional transfer functions can be calculated by a discrete fracture model or a dual-permeability, dual-porosity model at grid or cell scale (BSC, 2004, Appendix C).
2. Determine the particle residence time using the conditional transfer function of the continuum through which the particle will move eventually.

One note that two alternative grid scale conceptual model to represent fracture-matrix interactions can be used: dual-permeability/dual-porosity and a discrete fracture model. Figure G-2, taken from BSC (2004, Figure 7-12), suggests that the dual-permeability/dual-porosity model resulted in earlier predicted breakthrough curves for Tc-99.

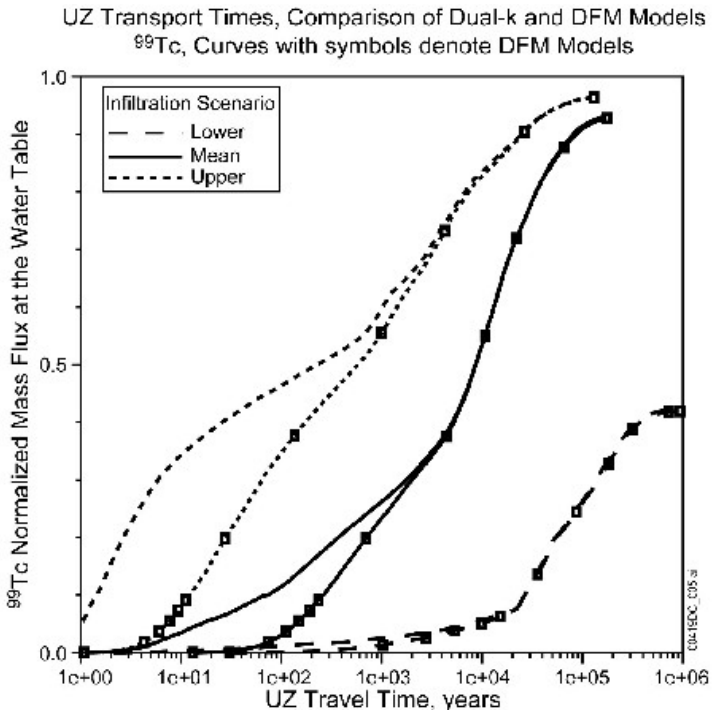
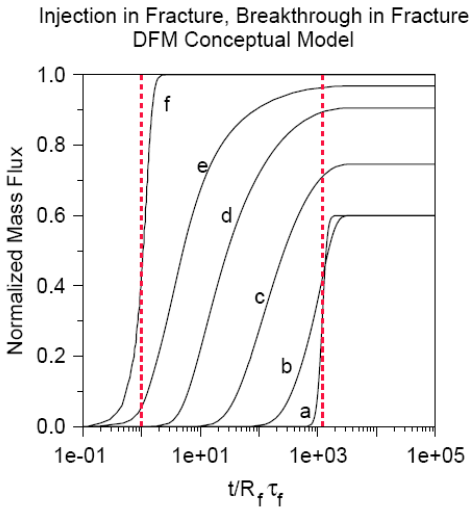


Figure G-2. Breakthrough curves of Tc-99 for three infiltration scenarios (BSC, 2004, Figure 7-12). Note that the model is the TSPA UZ transport model, but a uniform source across the repository and a fixed climate state is used for the individual calculations here.

The results shown in Figure G-2 reflect the differences in alternative conceptual models at the grid-scale, in particular, at intermediate matrix diffusion coefficients. Figure G-3(a) is the transfer function calculated using a discrete fracture model (from BSC, 2004, Figure C-1) and Figure G-3(b) is obtained by using a dual-permeability/dual-porosity model. Comparing curve c's in both figures, the dual-permeability/dual-porosity model suggests an earlier breakthrough than the discrete fracture model. However, the plateau of the two figures are roughly the same at 67%, indicating that probability of particle switching to the other continuum (vis-à-vis matrix diffusion) is not affected by the

conceptual model chosen at the grid scale. The difference is mostly at the sub-step 2, as suggested earlier, for particle residence times using either of the grid-scale conceptual models.

(a)



(b)

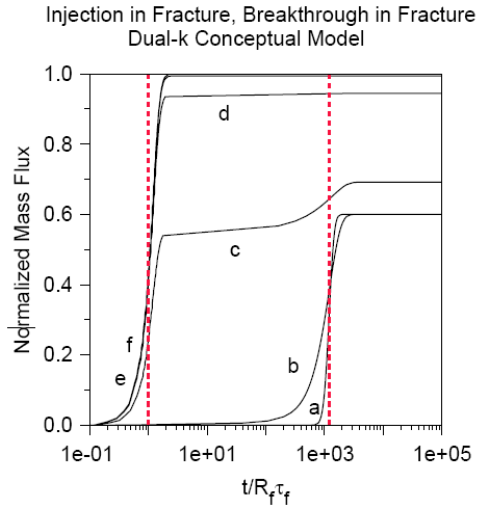


Figure G-3. Transfer functions calculated by using (a) a discrete fracture model and (b) a dual-permeability/dual-porosity model (from BSC, 2004, Figures C-2 and C-2).

References

BSC, 2004. Particle Tracking Model and Abstraction of Transport Processes WMDL-NBS-HS-000020 Rev 01, ICN 00, October 2004