HLWYM HEmails

From: James Winterle
Sent: Tuesday, October 10, 2006 10:18 AM
To: Hakan Basagaoglu
Subject: RE: about matrix diffusion
Attachments: DoE_approach_Oct_02_06-JW comments.doc

Hakan,
Attached is your review with my comments inserted in bold text.
--Jim

-----Original Message-----
From: hbasagaoglu [mailto:hbasagaoglu@cnwra.swri.edu]
Sent: Wednesday, October 04, 2006 3:07 PM
To: James Winterle
Subject: about matrix diffusion

James,

I've attached a brief write-up that lists my concerns about the way DoE has implemented matrix diffusion in their process level models.
I know you 're very busy with the TPA manual, but I would appreciate it if you could take a quick look at it -whenever you have some free time- and let me know
your thoughts on it. Thanks.

Hakan

Hearing Identifier: HLW_YuccaMountain_Hold_EX
Email Number: 504

Mail Envelope Properties (008001c6ec76$de335540$a5c8a281)

Subject: RE: about matrix diffusion
Sent Date: 10/10/2006 10:17:50 AM
Received Date: 10/10/2006 10:17:50 AM
From: James Winterle

Created By: jwinterle@cnwra.swri.edu

Recipients:
"Hakan Basagaoglu" <hbasagaoglu@cnwra.swri.edu>
Tracking Status: None

Post Office: cnwra.swri.edu

Files	**Size**	**Date & Time**
MESSAGE	628	10/10/2006 10:17:50 AM
DoE_approach_Oct_02_06-JW comments.doc	76864	

Options
Priority: Standard
Return Notification: No
Reply Requested: No
Sensitivity: Normal
Expiration Date:
Recipients Received:

Matrix diffusion in TPA and TSPA:

TPA Model:
Flow component: If the flow rate is greater than the fracture permeability, the flow will be fracture flow only. In TSw, no matrix diffusion was considered for the flow component.

Transport component: Matrix diffusion was not addressed.

TSPA Model:
They used an abstraction for the flow component. Predefined (or computed) flow field is used as an input to the transport component. The abstraction for the transport component is a 3D process-level model.

Questions/Concerns: [Note: Comments in bold below are made by Jim Winterle and represent an individual viewpoint, they are not necessarily a consensus viewpoint.]

1) In AMR2004 v02, DoE expressed the matrix diffusion (as diffusive flux into an infinitely large matrix storage) as a function interfacial area between a porous matrix and a fracture channel, which was considered to be a fitting parameter whose value was determined by fitting numerically calculated seepage values against the measured seepage rates -presumably- in the absence of dispersive transport in the fracture channel. Because they cannot measure the matrix-fracture interfacial area (a critical parameter for upscaling the matrix diffusion coefficient from a test scale to a field (mountain)-scale, (Liu et al., VZJ, 3:312-315)) independently for different layers within TSw, it appears to me that they can not quantify the matrix diffusion for different layers in TSw either, at least with their current model. If they can, how?

They cannot quantify it. It needs to be treated as an uncertainty and I believe that is what they do. In this case, our job would be to ensure the uncertainty parameter range that they select is reasonable and does not result in highly optimistic predictions of repository performance. In a case like this, we need to have an understanding of how much "credit" they get from the matrix diffusion process in their TSPA model.

There have been no conclusive remarks in their reports and journal articles on how to upscale the matrix diffusion coefficient from the fault-infiltration test at Alcove 8, Niche 3 (a test scale) to a field-scale at the Yucca Mountain? They proposed a fractal matrix-diffusion coefficient (with D=1.7 in their VZJ 2004 article) for the upscaling based on scarce data (Fig. 2 in their article). They did not discuss about the statistical confidence interval for their analysis? (it appears to me it would be very low). Considering scarcity of the data in their analyses (and other issues raised in #2 below), the proposed fractal dimension for the matrix diffusion, and the relevant upscaling (hence the argument on the significance of the field-scale matrix diffusion) remains still questionable. **As with many things in science and engineering, sometimes you have to make your best guess. We cannot dictate the approach they must take, but we can look at the range of uncertainty that is encompassed in their approach and make an assessment as to whether the results are too highly optimistic; generally, when uncertainty cannot be reduced without great expense (as may be the case here), the uncertainty range should encompass both the optimistic and pessimistic values with a mean that lies somewhere in between. Again, we also need to understand how much credit they are getting from matrix diffusion – does their safety case depend on taking this credit? I believe we have previously ranked this process as having "medium" significance to performance.**

2) Referring the fault test at Alcove 8-Niche 3 to analyze the significance of the matrix diffusion, I am not totally convinced if they really presented enough evidence for 'significance' of matrix diffusion in a 20-m deep vertical section in TSw at the test site:

They used two inert tracers (PFBA and Br) whose D_m's are on the same order of magnitude (on the order of 10^{-10}, and their D_m's are different only by a factor of 3) (Salve et al., WRR, 2004, 40, WR002571, p.3)). According to fig.7.6.9 of the AMR (and also in Fig. 9 of their WRR04 article), they noted that PFBA (with the lower D_m) arrived earlier and displayed a higher concentration peak. This might be considered as an indication for matrix diffusion (and apparently they did); but:

The arrival times and the peak concentration values of these two tracers were very close, and seem to be very difficult to make such a conclusive and strong statement from their analysis. I believe if they had plotted error bars (measurement errors, experimentalist usually do), the error bars from these two experiments might have overlapped. I would be convinced by their results if they showed that their experimental observations were actually repeatable (but, they reported results from a single experiment), or if they ran the experiment with different inert tracers whose D_m's are at least 2-3 orders of magnitude different (in this case the difference between arrival times and peak concentrations of two inert tracers would be much larger than potential measurement errors) (But, I do not know if there are two such inert tracers with D's 2-3 order of magnitude difference?).

Moreover, when they attempted to evaluate the effect of the matrix diffusion at the test site by looking at spread in BTCs of inert tracers, the matrix-diffusion coefficient was apparently treated/viewed as a lump parameter that includes the effects of fracture-matrix diffusion, fault-fracture channel interactions, fracture spacing, connectivity, and other properties. But, different configurations of fractures' connectivity and capillary barrier distributions at fracture junctions could theoretically result in spreads in BTCs even in the absence of matrix diffusion. So, the matrix diffusion may take place, but I do not see any strong evidence for the 'significant effects of matrix diffusion' as the author claimed in their WRR article and elsewhere.

Furthermore, even the authors were not consistent with their observations and interpretations in the same journal article (WRR04). In the last sentence of the paragraph # 29 on p. 10 of their WRR04 article, the authors, while referring to Fig. 9, stressed that "*because of the large temporal variability in tracer concentrations, it was difficult to discern whether PFBA BTC preceded Br at this locations*" referring to 2 out of 3 trays at the ceiling of Niche 3 (tray #6 and 9+23 (combined). But, then they referred to same figure in the first sentence of paragraph 40 on page 11, and noted that "*the tracer BTCs exhibit separation between Br and PFBA arriving earlier than Br in the arrival wave of the BTCs*". But, the latter was true only 1 out of 3 trays (tray # 7). They used the early arrival of PTBA as an indication of matrix diffusion for drawing a strong conclusion on the significant effects of the matrix diffusion, although they seem to be unsure about their observations.

If the entire case for matrix diffusion at Yucca Mountain was based on this one test, I might also be concerned. However, there are other field tests at Yucca Mountain (see Jude McMurry's report), there are numerous laboratory experiments and many years of scientific research on the process of matrix diffusion. It would be very difficult to argue that matrix diffusion does not occur in any environment where there is a chemical potential gradient between a fracture and a porous matrix.

Apart from this:

They used 20-fold less PFBA mass than li-Br in their tests (no explanation for why?), and noted in the end of the experiment that PFBA arrived in earlier than Br (Salve et al., WRR, 2004, 40, WR002571) (which is not clear to me from Fig. 9 in their article). When the initial concentration of Br was higher that that of PFBA, the Br would be "forced" to diffuse into the matrix (or possibly into smaller dry fractures, stagnant water, dead-ended fractures, cavities) more due to the high concentration gradient across the matrix-fracture interface, when the initial concentrations of these inert tracers are presumably zero (or the same) in the system (according to paragraph # 38 on p. 11), fractures and faults are probably initially dry and background bromide concentration is zero). In this case, more Br is expected to be diffused into the matrix or other fractures and hence

it will have a delayed and possibly small peak in its BTCs, as they observed from their experiments. But, this is NOT because PFBA has a smaller D_m. because they seem to obscure the effect of D_m by higher concentration gradients. **The initial concentration of PFBA should not matter at all other than it needs to be sufficient to be detected by the instruments they are using (I believe PFBA is very easy to detect in small quantities). The analytical methods used are based on normalized concentrations; the initial concentration does not change the result.**

Although they presented the resulting BTCs in a dimensionless form, Br will more likely be lost to small fractures and slower fracture paths (when Br and PSBA compete for the same site); therefore, the transport time of Br is to be delayed a bit, and its peak concentration will be a slightly lower. **Not true! Perhaps more total mass may be transferred, but relative to its initial concentration, there will be no bias in the normalized results. Of course Br will diffuse faster because it is a smaller molecule, but that was the whole point of the experiment.**

3) With regard to the conceptualization, in the aforementioned AMR, the two units in TSw were identified with different hydraulic properties (e.g., fracture spacing (frequency), matrix porosity, etc.). All these properties were assumed to be uniform in each unit while their average values were assigned to the hydraulic properties of the fault (for the fault infiltration analyses). In large plot analyses, all columns (a total of 12) were assumed to have different hydraulic properties than the rest of the host rock, although the hydraulic properties were presumably remained the same in each subunit along each column. Whereas in 2002 (Salve et al.) paper, the units were split into High-Permeability Zone (HPZ) and LPZ (that were 1 m apart). In their numerical analyses, only injection through HPZ resulted in seepage at the niche/slot ceiling unlike water injection through LPZ. After all, which conceptual model will be adopted in their final analyses? **If the "final analysis" is the TSPA model, probably neither conceptual model will be adopted. We do not need to be too concerned with how they decide to interpret their data. In the end, the conclusions will likely be the following: (1) there is "probably" at least "some" degree of matrix diffusion that occurs; (2) the actual amount of matrix diffusion is highly uncertain because of difficulties in constraining model parameters and boundary conditions; and (3) this uncertainty will be very difficult or impossible to reduce in any such large scale field test; (4) because of this irreducible uncertainty, it is appropriate to consider a range of possible parameters in a TSPA model; and (5) that range of uncertainty in TSPA should be based on the body of available scientific data in addition to the single A8-N3 test.**

4) They noted (Seol YS, Liu HH, Bodvarsson GS, GRL, 30(2), p. 1075, 2003) that if simulation models do not consider the effects of dry fractures (and hence the degree of matrix-matrix connection, which control the capillary and diffusive barriers) may *underestimate* radionuclide travel times through the UZ of YM. However, they have not discussed the potential effects of dry fractures (and hence the connection of matrix-blocks) in quantifying the matrix diffusion at Alcove 8 niche 3 (re: the fault infiltration experiment)? **Perhaps this may be because the A8-N3 test was conducted under ponded conditions and the fractures that carried the water were relatively wet compared to the ambient conditions that Seol et al were describing. Even if they did not discuss effects of dry fractures in the A8-N3 test, did their model not include area reduction factors and the active fracture parameters which are used to account for the effects of non-flowing fractures?**

5) Fracture frequencies used for Tsw34 was reported to be 1.72 m^{-1} in AMR (p. 7.20), whereas it was reported as 1.50 m^{-1} by HH Liu et al. JCH 745. p45 (2004). and by Zhou et al. (2006 JCH; 87; p.99). Why? Any technical basis (or field observations) for such changes? **In hydrology, 1.72 and 1.50 might be considered an exact match! In reality fracture frequency is much higher because the only counted fractures with trace lengths above a certain cutoff. It doesn't really matter, though. In my own opinion, fracture frequency measurements are meaningless for this type of analysis and we are wasting out time thinking about them; the only question related to fractures that needs to be asked is the following: Are there**

enough interconnected fractures that the system can be modeled as a dual-permeability or dual-porosity continuum? At Yucca Mountain, I would maintain that this answer is clearly YES for any scale larger than about 1 or 2 meters.

6) The active fracture parameter was reported to be (after model calibration) 0.426-0.44 (in Liu et al., WRR, 34(10), 1998 p.2640), whereas it was taken as 0.41 (considered as an initial guess, based on Ahlers et al., 2000, but this initial guess was remained unchanged in their numerical analysis) by Liu et al. JCH, 74, 2004, p. 49. Why they decided not to use their earlier estimate (in Liu et al., 1998) for the active fracture parameter? This may not be an issue, if the fracture saturation exceeds 0.5. However, when fracture saturation less than 0.5, the number of active fractures will be 2-7% less when γ =0.44 than when γ =0.41 for water saturation is less than 0.5. The percent difference in number of active fractures can be as high as 4-13% when γ =0.5 than when γ =0.41 (They used in one of their report γ >0.5). **See my comment for item 3.**

	Active Fracture Parameter				ABS(Percent Differences Wrt 0.41)		
Saturations	0.41	0.44	0.5	0.55	0.44	0.5	0.55
0	0	0	0	0			
0.1	0.389045	0.363078	0.316228	0.281838	6.67457	12.90364	10.87491
0.2	0.516919	0.492553	0.447214	0.412635	4.713604	9.205028	7.731917
0.3	0.610407	0.588753	0.547723	0.515723	3.547467	6.969089	5.842252
0.4	0.686823	0.6682	0.632456	0.604134	2.711435	5.34935	4.47809
0.5	0.752623	0.737135	0.707107	0.68302	2.05797	4.073588	3.406367
0.6	0.81104	0.798705	0.774597	0.755063	1.520794	3.01846	2.521786
0.7	0.863953	0.854758	0.83666	0.821872	1.06432	2.117313	1.767567
0.8	0.912571	0.906483	0.894427	0.884503	0.667195	1.329938	1.109517
0.9	0.957722	0.9547	0.948683	0.943699	0.315583	0.630169	0.525417
1	1	1	1	1	0	0	0

7) In a recent article by Zhou, Liu, Gudmundor, Bodvarsson, and Molz (Transport in porous media, 2006, 63:473-487), it was noted that "the multi-process (I would rather call it multi-zone that involves different zones with different D_m's) model is more representative of the matrix diffusion process involved in the tracer test than the single-process model" (the latter was assumed in fault and large plot infiltration tests at Alcove 8-niche 3 to quantify the matrix diffusion) (p.481). They also noted that, at different scales, the different tracer transport behavior is obtained using different transport model" (single vs multi-process model) (P.484). After all, based on their conclusions, the use of single process model (with a single D_m value for the entire matrix that would presumably represent the most dominant/characteristic diffusion process) for the quantification of matrix diffusion at the test site cannot be representative. Besides, the field test (at a relatively smaller scale) was conducted to gain insights into the effects of matrix diffusion on the overall radionuclide transport on a larger scale (mountain-scale). However, the authors noted that as the spatial scale changes by an order of magnitude, the single and multi-process models can produce substantially different results. So, are they going to revise their conceptualization, analyses, and interpretations on the matrix-diffusion (so far based on a single process model) in accordance with their new insights and numerical findings? **Ah! Are they are planning to change their conceptualization in the TSPA model? If so, this is something I did not know and something we need to watch very closely. The question we need to stay focused on, however, is not they choose to interpret any individual test. I believe the most important conclusions from these analyses will remain unchanged, which as I mentioned earlier, are that matrix diffusion is probably occurring to at least some small degree, and that the overall amount of diffusion mass transfer at the mountain scale will**

be highly uncertain. Therefore, the major question we must focus on is whether this irreducible uncertainty is incorporated into the TSPA model.