HLWYM HEmails

From: Paul Bertetti
Sent: Tuesday, April 24, 2007 10:56 AM
To: jwinterle@swri.edu
Cc: Jude Mcmurry; Ronald Janetzke
Subject: RE: Glitches from Test Case P12-3 (UZFT)

Jim,

Yes, the surface area calculation was not checked directly. We will need to redo the spreadsheet so that the correct values for the calculated surface areas appear and can be compared to a hand calculation. I will take care of generating a new version once the changes are in place.

After working on this issue yesterday (I was sure that we had discussed this problem in Aug 2004 -- and we did), I discovered the oversight came from a misunderstanding in the implementation of SCR-517. SCR-517 has an attached file where I described the problem with bulk vs. grain density, and it is noted explicitly in the change request. However, when the other changes were made to the code, the bulk density portion was not implemented because of the use of bulk density in the Rd subroutine (as noted in the SCR) must have confused Femi (it could have been written up more clearly by me). Obviously, I did not follow up on the expected change at the time, and the code was never updated as I had expected. Since I assumed (incorrectly) that the code had been changed, I did not think to check the ssarea calculation later. I do not have a reasonable explanation as to why I did not 'catch it' for the next three years. Fortunately, Jude was paying attention.

Paul

-----Original Message-----
From: James Winterle [mailto:jwinterle@swri.edu]
Sent: Tuesday, April 24, 2007 9:34 AM
To: jude.mcmurry@swri.org; 'Ron Janetzke'; 'Paul Bertetti'
Subject: RE: Glitches from Test Case P12-3 (UZFT)

All:

Regarding item 1. I double checked through the uzft.f code and it does appear to be an error that should be corrected. Interestingly, when you make this correction, the grain density, matrix porosity, and the (1-grain density) factors all cancel out when the Kd is converted to an Rd. So, this abstraction could actually be made much simpler since the only terms that don't cancel out are the Ka and the pore radius. However, given the schedule, I think it would be safer and easier to just make the change suggested by Jude.

Paul, for the SZFT validation, I am using the spreadheet that you provided last year for version 5.1betaD. Under the tabs titled "Alluvium" and "STFF_matirx," the numbers reported for hand calculations and tpa calculations are identical. But I'm assuming this was based on trusting the Kd and density values reported by TPA. I'm about halfway through writing this up for the validation test, so, do we need to redo this spreadsheet with TPA version 5.1betaW? I suppose we will have to wait for the fix, which I hope can be done by late this week or early next week.

Ron,
Let me know when this has been assigned an SCR.
--Jim

-----Original Message-----
From: Jude McMurry [mailto:jmcmurry@swri.edu]
Sent: Monday, April 23, 2007 5:00 PM
To: James R Winterle; 'Ron Janetzke'
Cc: 'Paul Bertetti'
Subject: Glitches from Test Case P12-3 (UZFT)

Jim and Ron,

While running the UZFT validation test P12-3, I found several glitches related to the calculation of actinide Kd's and to how Kds and Rds are reported in uz_kdrd.out. Similar glitches are also present in SZFT (at least for the fractured tuff layer).

(1) The main problem is that the code is using the wrong term to calculate effective surface area ("ssarea"), which is used with Ka values (determined from coefkdeq.dat) to calculate the actinide Kds. The formula uses rock grain density instead of rock bulk density in the surface area calculation. The attached file shows what needs to be amended in the equation.

(2) One aspect of test P12-3 was to confirm that UZFT is writing matrix Rds to the intermediate file uz_kdrd.out. It is not. The matrix Rd values are being calculated and used in transport calculations, but they are not getting listed in the uz_kdrd.out file (note the blank spaces in the columns). Another problem with this intermediate output file is that uz_kdrd.out is only reporting the Kd and Rd data for five of the six actinides (Am, Np, Pu, Th, and U). The data for Cm needs to be reported here, also.

(3) For clarity, some of the comment lines in the code probably should be updated so the reader will understand that Kd and Rd values are calculated for six actinides (Am, Np, Pu, Th, U, and Cm) instead of five. I searched the uzft.f file and identified about 8 or 9 lines of commented text that should be revised, as shown in the attached file.

Jude

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