HLWYM HEmails

From: Paul Bertetti
Sent: Thursday, May 19, 2005 5:29 PM
To: Tina Ghosh
Subject: FW: TPA/nefmks validation

Tina,

I am really behind on a lot of things, so I am a little late in responding to your and Scott's request.

It's hard to tell what folks mean by before. In previous versions of TPA (4.x), Kds or Rfs were specified through individual (each element) distributions. For TPA 5.x, the Kds for five actinides (Am,Np,Pu,Th,U) are treated differently, the remainder of the radionuclides, including other actinides such as Cm, have their Kds/Rfs sampled directly from distributions - most of which have been converted to constant values. We've been testing 5.x for some time so most refer to activities like RARI as "before".

For the big five, pH and CO2 are sampled from distributions in the TPA input file (NOTE: the distributions are outdated and should be changed before we validate - I have sent the revised information to Ron Janetzke). CO2 is sampled first (independent) and pH (dependent) is correlated to CO2. Using the CO2 and pH values, coefficients representing a 5th-order polynomial are selected and used to calculate a Ka. Sampled or calculated surface area values are then applied to the Ka to determine the Kd (and an Rf eventually). The 5th order polynomial is simple:

$$y = a + bx + cx2 + dx3 + ex4 + fx5$$

where y = Ka, and x = pH. The coefficients are found in the coefkdeq.dat file. There is a separate set for differing values of CO2. Note that the code interpolates the coefficients for values of CO2 that are in-between those listed. CO2 and pH values sampled outside the ranges listed should produce Ka values of zero.

For the validation exercise I would like to review output from a multiple realization run to compare TPA-produced Ka values with the model Ka envelope. I would also want to check the pH and CO2 correlation and check operation for input values that are outside the range currently provided in the input file. I would also like to compare the distribution of Kas/Kds/Rfs with independently produced distributions from GoldSim.

Hope this helps.

Paul

-----Original Message-----
From: Scott Painter [mailto:spainter@cnwra.swri.edu]
Sent: Monday, May 16, 2005 4:32 PM
To: Paul Bertetti
Subject: FW: TPA/nefmks validation

Paul,

I've already answered (1) but I can't answer number (2).

Scott

-----Original Message-----
From: Tina Ghosh [mailto:STG1@nrc.gov]

Sent: Monday, May 16, 2005 3:57 PM
To: spainter@cnwra.swri.edu; Timothy McCartin; oosidele@swri.org
Subject: Re: TPA/nefmks validation

Dear Scott,

A couple of questions:
(1) for nefmks: You mentioned last week that NEFTRAN has been modified to handle different diffusion coefficents for different radionuclides. Is this implemented through nuclide-specific modifiers to the base diffusion coefficient? Where could we find the relevant input/calculations/output?
(2) for uzft/szft: Is the dependence of Ka on pH implemented the same as before (through a look-up table)? Could you send us the relevant equations/tables?

Thank you very much for any assistance.

Hope all is well,
Tina

>>> Scott Painter <spainter@cnwra.swri.edu> 05/06/05 09:53AM >>>
All,

I'm willing to take the lead on the nefmks validation task. It is my understanding that we can limit the validation to my recent modifications, which were very minor.

Scott Painter

Hearing Identifier: HLW_YuccaMountain_Hold_EX
Email Number: 1097

Mail Envelope Properties (pbertetti@cnwra.swri.edu20050519172900)

Subject: FW: TPA/nefmks validation
Sent Date: 5/19/2005 5:29:27 PM
Received Date: 5/19/2005 5:29:00 PM
From: Paul Bertetti

Created By: pbertetti@cnwra.swri.edu

Recipients:
"Tina Ghosh" <Tina.Ghosh@nrc.gov>
Tracking Status: None

Post Office:

Files	**Size**	**Date & Time**
MESSAGE	3315	5/19/2005 5:29:00 PM

Options
Priority: Standard
Return Notification: No
Reply Requested: No
Sensitivity: Normal
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