HLWYM HEmails

From: Paul Bertetti
Sent: Tuesday, March 01, 2005 1:28 PM
To: Christopher Grossman
Subject: RE: Review of TPA input file parameters

Chris,

Your questions are good ones, and I do not have a quick set of answers. In some cases, use of expected values as constants will likely be sufficient. There are a couple of nuclides in DOE's TSPA (e.g., Sr) that are not included in TPA. I would hope that we can use the information I provided as a guide for making some decisions about these parameters. I am not certain how best to proceed.

Paul

-----Original Message-----
From: Christopher Grossman [mailto:CJG2@nrc.gov]
Sent: Monday, February 28, 2005 3:16 PM
To: pbertetti@cnwra.swri.edu; Hans Arlt; John Bradbury
Cc: dpickett@cnwra.swri.edu; dturner@cnwra.swri.edu; epearcy@cnwra.swri.edu; jmcmurry@cnwra.swri.edu; jwinterle@cnwra.swri.edu; oosidele@cnwra.swri.edu; rjanetzke@cnwra.swri.edu; spainter@cnwra.swri.edu; Bret Leslie; Timothy McCartin
Subject: Re: Review of TPA input file parameters

Paul-

Thanks for putting together this monumental task. I only have a couple of considerations regarding the tpa.inp file parameter update:

1) A number of the parameters that were flagged for update with new distributions were formerly constants. Changing these parameters to distributions will require sampling operations by TPA and would be expected to add a significant burden to TPA calculations (in the form of run-time, correlation issues, and confounding effects on determining sensitive parameters). My suggestion would be to perform sensitivity analyses (either prior to making the changes or, rather, if we perform system-level analyses after the code is completed) or use existing analyses to determine which of the parameters that are being considered for a change from constant to distribution would, in fact, need to be changed to a distribution based on impacts on system-level risk. Those parameters that do not have a significant impact could simply remain constants with a value equal to the expected value from the new distributions. We should probably discuss what the best approach to this might be.

2) I noticed a few of the parameters flagged for update were for radionuclides not evaluated by DOE's TSPA. Are these radionuclides significant? If not, can they and their associated parameters be removed from the code? Also, there may be some radionuclides that DOE is evaluating and we, currently, are not in TPA. Even though they may not be risk-significant radionuclides, we may want to consider adding them to enhance our ability to review DOE's TSPA-LA.

Chris

>>> Paul Bertetti <pbertetti@cnwra.swri.edu> 02/25/05 03:18PM >>>
Hans and others,

After much delay, I have completed an initial review of what I feel are relevant TPA parameters for RT in the SZ (and UZ). I have tried to provide comment for all the parameters I reviewed. It is my opinion that many parameters need to have their value range and distributions updated. This opinion is based on input from many folks including Dave Turner (please see his suggested changes spreadsheet) and Jude McMurry as well as discussions with a number of you along the way. I thank all for you patience with me and for your discussions to this point. In the attached spreadsheet I have added a comment column, a recommended contact person (where changes should be made), and an indication of no change or a new value range where needed. I have added color to some cells to indicate the status of the recommended change. Green indicates that the new range recommended is currently supported by the information I provide in the comment field. Orange (or whatever color that is) indicates changes are required, but work to finalize the numbers is not yet complete. Items requiring no change (in my opinion) are left white.

I ask each of you to review the annotated spreadsheet. Review the suggested changes and no change recommendations. Ask questions and discuss as needed to develop an understanding and consensus for these values. We can then proceed to make Ron's life even busier by requesting the changes be implemented into TPA.

In response to the two questions on Wednesday's e-mail:

1. What additional changes to the code are necessary?

For RT items, (i) the input file should be update to reflect the changes I have listed once final values are agreed upon by all, (ii) the modification to the code to implement the colloid-facilitated transport model must be completed and tested, (iii) any additional work to implement or modify NEFTRAN for diffusion of colloids and use of dissuasion in the UZ should be completed, (iv) work to ensure the code is capable of producing lists of intermediate calculated values (e.g., surface area of a layer, sampled Ka, etc.) must be completed to ensure a reasonable way of error checking and verifying the code, and (v) changes to the coefkdeq.dat file must be completed for all nuclides.

Ron and his team have been working hard on number (iv) for some time, but changes in scope and schedule have caused delays. I think it is extremely important that such error checking code be completed to facilitate verification of intermediate calculations for all RT related items.

2. What are we doing?

A. We continue to perform a detailed review of input parameters to try to understand the uncertainties that are or are not incorporated in TPA as a result of using certain values. For instance, porosity of UZ layers is an important term in the calculation of Rf from Kd. Is the constant value appropriate (probably so), is ignoring the distribution of porosity for each layer important? Additional work to finalize values and ranges is also in progress. All value and ranges for TPA input files and supplemental files (like coefkdeq.dat) will be finalized by the March deadline.

B. We are conducting field and experimental studies of sorption onto alluvial materials. Evaluation of sorption in the alluvium is important. We would like to compare TPA predicted values based on models of previous experiments to values measured on actual alluvial materials using actual alluvial groundwater. The experiments are underway. We will be collecting some samples from the 22 sonic core in a couple of weeks and will analyze those samples in detail. Important parameters like alluvium surface area are based on limited information form 19PB. The 22 data will help to corroborate our information and conceptual models. This work will proceed through the end of the fiscal year and likely beyond. Any new or relevant information will be used to understand the strengths and weaknesses of the current TPA model.

C. Process-level modeling will continue to evaluate colloid transport issues, evaluate requirements for confirming experiments, and evaluate aspects of kinetic controls on Np sorption. Although these activities are indirectly related to TPA, they will help to bound our current conceptual models of transport.

D. Additional work to review and analyze input parameters will continue beyond March. This work will focus on items such as Np species log Ks that have been updated by NEA. Do the updates significantly affect our model predictions? Other items include confirmation of Am sorption values and review of Th complexation. This work is ongoing and will occur as time permits. If TPA changes are warranted, appropriate notifications will be made.

Should you have any questions or require further information please do not hesitate to contact me (210-522-5228).

Paul

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