Scientific Notebook No. 170E: Total Performance Assessment (TPA) 3.2 Development (April 3, 1996 through September 16, 2003)

SCIENTIFIC NOTEBOOK

170-13E

Printed: March 23, 2005

Patrick LaPlante SCIENTIFIC NOTEBOOK No. 170-13e
INITIALS:__PL____

SCIENTIFIC NOTEBOOK #170-13E

Documentation of TPA Code Work

by

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September 11, 2000

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Printed: March 23, 2005

Patrick LaPlante SCIENTIFIC NOTEBOOK No. 170-13e
INITIALS:__PL____

[Patrick LaPlante, September 11, 2000]

Title: Recalculation of DCFs for DCAGS Using Updated Mean Value Consumption Rates

Participants: Patrick LaPlante

Objective: Update TPA dose conversion factor (DCF) tables in DCAGS module to maintain consistency with updated consumption rate parameters used in DCAGW.

Work Plan:

– Obtain GENII-S (v1.485) input files (ascii format) used for calculation of DCFs for TPA 4.0 related to food consumption (i.e., animal product consumption and crop consumption). These files are named S30CBTR1, S30CBTR2, S30CBAN1, and S30CBAN2 and have *.inp and *.flg extensions. Files are dated 5/31/98 for the files ending in '1' and 9/28/98 for files ending in '2'.

– Use GENII-S code to edit the consumption rate parameters for crops and animal products to fixed values from the DOE sponsored food consumption survey of Amargosa Valley (a summary of the survey results is found in the DOE Analysis Model Report entitled "Identification of the Critical Group (Consumption of Locally Produced Food and Tap Water)" ANL-MGR-MD-000005, Rev. 00). Check other parameters in the input file to ensure consistency with TPA version 4.0 input file for GENTPA (ggenii.inp) to ensure all other biosphere and critical group parameters used for DCAGS DCFs that are used for ingestion dose calculations from a soil source concentration are compatible with the comparable parameters used in DCAGW. In TPA version 4.0 there were some minor consistency changes and this check will ensure the two modules (DCAGW and DCAGS) use DCFs based on similar biosphere and critical group assumptions. (updated input files are STP41TR1, STP41TR2, STP41AN1, STP41AN2 with *.INP and *.FLG extensions).

– Run an unmodified input file from TPA 4.0 DCF calculations to compare with the corresponding TPA 4.0 DCFs to confirm the GENII-S setup has not been changed since the last time the code was used (files are S30CBTR1 .INP .FLG and .OUT and comparison of results is in excel97 file S30CBTR1.QACOMP.XLS).

– Run GENII-S with the updated input files and tabulate results in Excel97 spreadsheet files (ascii format output files named same as input files with *.OUT extension and Excel97 file is TP41SOIL.XLS).

– Because GENII-S dose output includes daughter ingrowth, use spreadsheet to sum daughters and add to each parent dose (Excel97 files SUMDTR41.XLS, TP41SFNL.XLS)

– Reorganize GENII-S dose output on spreadsheets to order of radionuclides specified in the TPA DCF data files, import columns of unchanged data from existing TPA DCF data files, convert spreadsheet to ascii text, then cut/paste all data into TPA DCF data file and edit header to reflect changes in data (files gs_cb_ad.dat; gs_pb_ad.dat). Pluvial ingestion DCFs for the soil source in gs_pb_ad.dat are the same as in

PATRICK LAPLANTE SCIENTIFIC NOTEBOOK NO. 170-13E
INITIALS: PL

Title: Documentation of the TPA 4.1 Testing: Leach Factor Calculation Modification for DCAGW.

Participants: P. LaPlante

[Patrick LaPlante, September 26, 2000]

Objective: Confirm the modified equation for the leach factor in DCAGW has been implemented correctly (SCR-325, Attachment 2 testing).

Work Plan: The leach factor calculation in DCAGW has been modified to include a volumetric water content term in the numerator of the equation (the infiltration rate in the numerator is now divided by the volumetric water content). In TPA the results of the leach factor calculation are written to a data file (gftrans.inp). Thus, the modified calculation will be tested by comparing the results in the gftrans.inp file from a TPA 4.1 code run with results of a hand calculation (excel spreadsheet) using the same equation and input parameters. To account for rounding errors, a maximum deviation of 5% will be allowed between the results being compared.

Results/Discussion: The hand calculation is provided on an excel spreadsheet (leaccalc41.fin.xls). Parameters used for the hand calculation are provided in the spreadsheet. Because the spreadsheet was created first, any parameters that were different than the default values in tpa.inp were changed in tpa.inp to be consistent with the spreadsheet (e.g., Kd's). The comparison of the hand calculations with the values output from tpa (in gftrans.inp) on the spreadsheet indicate good agreement . None of the values differed by more than 2%, which is expected to be due to differences in rounding results. The comparison was done for only those radionuclides where the TPA code allows user input of Kd's for the leach calculation. The calculated leach factors were also compared with the TPA 4.1 default leach factors (from gftrans.def) to show that the hand calculated factors were different. This was done because if the test had merely duplicated the the 4.0 results, there would be no objective evidence to confirm that the calculation of leach factors within TPA was being used by the code to generate the results in gftrans.inp. Because the results of the hand calculation agreed with the TPA code results, the code passed the test.

[Patrick LaPlante, March 29, 2001]

All files referenced in the results/discussion section are provided on the attached floppy disk (labeled Scientific Notebook #170-13e Files, subdirectory SCR325ATT_2).

gs_cb_ad.dat because the GENII-S model does not account for leaching (the only effect of water balance changes on the dose) if a soil concentration is the source of contamination (as is modeled for the DCAGS DCFs).

– Compare new DCFs with the prior set of TPA 4.0 DCFs to document the magnitude of changes due to the changed input parameters (file is Excel97 format S30CBTR1.QACOMP.XLS).

[Patrick LaPlante, September 18, 2000]

Results/Discussion:

The resulting updated DCFs are provided in new data files for TPA (ascii format gs_cb_ad.dat, gs_pb_ad.dat). The changes to the DCFs due to new consumption rate information have lowered all except one value which was increased by 20% (Tc99) due to an increase in the average leafy vegetable consumption rate. All other DCFs were lowered from between 10 and 90% due to lower consumption rates for the food products that dominate each radionuclide-specific DCF. The lowering effect varies with radionuclide because each radionuclide's effect on dose is influenced to varying degrees by a variety of exposure pathways related to ingestion of contaminated foods (e.g., some radionuclides concentrate more readily into certain foods than others).

[Patrick LaPlante, March 29, 2001]

Attachments: Floppy disk labeled "Scientific Notebook #170-13e Files" with all referenced files in subdirectory SOILDCF.

Printed: March 23, 2005

Patrick LaPlante SCIENTIFIC NOTEBOOK No. 170-13e
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[Patrick LaPlante, September 26, 2000]

Title: Documentation of the TPA 4.1 Testing: Leach Factor Calculation Modification for DCAGW.

Participants: P. LaPlante

Objective: Confirm the modified equation for the leach factor in DCAGW has been implemented correctly (SCR-325, Attachment 2 testing).

Work Plan: The leach factor calculation in DCAGW has been modified to include a volumetric water content term in the numerator of the equation (the infiltration rate in the numerator is now divided by the volumetric water content). In TPA the results of the leach factor calculation are written to a data file (gftrans.inp). Thus, the modified calculation will be tested by comparing the results in the gftrans.inp file from a TPA 4.1 code run with results of a hand calculation (excel spreadsheet) using the same equation and input parameters. To account for rounding errors, a maximum deviation of 5% will be allowed between the results being compared.

Results/Discussion: The hand calculation is provided on an excel spreadsheet (leaccalc41.fin.xls). Parameters used for the hand calculation are provided in the spreadsheet. Because the spreadsheet was created first, any parameters that were different than the default values in tpa.inp were changed in tpa.inp to be consistent with the spreadsheet (e.g., Kd's). The comparison of the hand calculations with the values output from tpa (in gftrans.inp) on the spreadsheet indicate good agreement . None of the values differed by more than 2%, which is expected to be due to differences in rounding results. The comparison was done for only those radionuclides where the TPA code allows user input of Kd's for the leach calculation. The calculated leach factors were also compared with the TPA 4.1 default leach factors (from gftrans.def) to show that the hand calculated factors were different. This was done because if the test had merely duplicated the the 4.0 results, there would be no objective evidence to confirm that the calculation of leach factors within TPA was being used by the code to generate the results in gftrans.inp. Because the results of the hand calculation agreed with the TPA code results, the code passed the test.

[Patrick LaPlante, March 29, 2001]

All files referenced in the results/discussion section are provided on the attached floppy disk (labeled Scientific Notebook #170-13e Files, subdirectory SCR325ATT_2).

Printed: March 23, 2005

Patrick LaPlante SCIENTIFIC NOTEBOOK No. 170-13e
INITIALS:__PL____

[Patrick LaPlante, August 27, 2001]

Title: Documentation of the TPA 4.1d Runs to Support Response to Peer Review Question Regarding Potential Non-conservativeness of TPA Residential Receptor Exposure Pathways.

Participants: P. LaPlante

Objective: Estimate the Potential Magnitude of Change in TPA 4.1d Residential Receptor Dose from Addition of Exposure Pathways

Work Plan: A TPA peer review comment (comment #81) questioned that the residential receptor scenario was non-conservative because it limited exposures to the drinking water pathway. The commenter noted that it was reasonable to assume a residential receptor may purchase foods from Amargosa Valley or have a garden that could produce crops for personal consumption. Because the TPA code does not have the flexibility to add exposure pathways to the residential receptor, a bounding calculation using TPA 4.1d was done. This calculation involved running the base case tpa.inp file for a residential receptor to determine which radionuclides dominate the residential receptor dose (file:Peer81\stochbaseresident\ rgwna.tpa charted in avgdosenuc.xls). Then, exposure-specific DCF output (file: Peer81\meanvalue20km\gw_cb_ad.dat) from running the base case at 20km (the location where all pathway calculations are performed), mean value input file (Peer81\meanvalue20km\tpa.inp) was compiled on a spreadsheet (file: Peer81\meanvalue20km\pathwayfrac.xls) to estimate the fraction of the total dose for each pathway. The sum total of pathway fractions for all non-drinking water pathways for important radionuclides were used to estimate the magnitude increase in the total dose expected if the exposure pathways were included in the residential receptor calculation.

Results/Discussion: Results are summarized below in the response to the peer review comment. In short, Because Np-237 dominated the residential receptor dose, and drinking water contributes about 54% to the mean value, all pathway, 20km dose calculation for that radionuclide, addition of all the non-drinking water pathways to the residential receptor location is expected to be no greater than approximately double the residential receptor dose. Because it is unlikely all the 20km location (farming) pathways would be relevant to the resident, the magnitude of total dose increase from addition of only the pathways relevant to the resident is likely to be less than the factor of two found in these results.

Response to Peer Review Comment:

The residential receptor was defined as an alternative for perspective only. Both NRC and EPA have defined the critical group (now reasonably maximally exposed individual or RMEI to conform to EPA regulations) as a farming group at 18 km as the most highly exposed group based on current conditions to limit speculation about potential future behaviors. Using current conditions for the RMEI definition is a matter of NRC policy that is consistent with the recommendations provided to the NRC and EPA by the NAS committee on YM regulations. Nonetheless, to add perspective to the concern that doses might be significantly higher for the residential group with added pathways consider the following results of TPA code

calculations. If the residential receptor dose were to include the same suite of exposure pathways as the 20 km group (e.g., crop and animal consumption) the highest expected annual dose (at 10,000 yrs) would likely only increase by a factor of about two. This is because the dose is dominated by Np-237 (see file: avgdosenuc.xls) and the drinking water contribution to the dose for this radionuclide at the 20 km farming location is about 54% (see pathwayfrac.xls)(therefore, adding the other pathways to the residential scenario would increase the dose by about two times). This estimate is expected to be an upper bound on the increase in groundwater pathway dose to the residential receptor due to addition of the suggested pathways and it is likely an actual resident would have fewer exposure pathways than the farmer and thus the dose is more likely to be between the current drinking water only scenario result and two times that value. Given the residential group is much more speculative than the farming group (i.e., no current residents live that close to YM) and the magnitude of the change in dose is not great, the farming critical group is considered to be a reasonable choice for calculating doses. More information on the selection of the RMEI is provided in the federal register notice for 10 CFR Part 63.

Referenced Files:

All files referenced in the work plan and results/discussion sections are provided on the attached floppy disk (labeled Scientific Notebook #170-13e Files, subdirectory Peer81).

[Patrick LaPlante, October 2, 2001]

Note that the dates on pages 1-7, and hereafter, may not all be consecutive because comments have been inserted after the original text of the writeup was written. These comments are analogous to margin comments written and signed/dated in a hard copy notebook. In all cases, the dates apply to the text that follows until a new date appears which then applies to the following text...and so on. Those instances in the prior pages where dates are not consecutive are due to inserting the comments that point to the floppy disks that contain the referenced files. While the files were created when the work was initially done, the floppy disks collecting the files on one media for record keeping purposes were created and noted in the notebook comments when the notebook was submitted for the 6 month review rather than at the time the technical analysis was documented.

Patrick LaPlante SCIENTIFIC NOTEBOOK No. 170-13e
INITIALS:__PL____

[Patrick LaPlante, October 24, 2002]

Title: Hand Calculation to Verify Implementation of Updated Groundwater Protection Calculations in TPA 5.0 Beta Code.

Participants: P. LaPlante, M. Smith

Objective: Verify calculations for groundwater protection in TPA 5.0 beta version are being executed correctly by comparison with spreadsheet calculations using input data and mathematical computations that are identical to the TPA code implementation.

Work Plan:

The overall approach for conducting the hand calculations will be to execute a TPA 5.0 base case single realization run with the mean value input file that has been modified to increase the number of radionuclides released and transported to groundwater for testing purposes. Selected input data, intermediate results, and output from the modified base case run will be used to populate a spreadsheet that contains the conversions to results consistent with groundwater protection requirements. Agreement between output from the spreadsheet calculation and output from TPA code will demonstrate that calculations are being implemented correctly in TPA 5.0 beta version. Detailed steps of the work plan follow:

1. Use the TPA 5.0 beta code to generate a mean value input file for the base case. Modify the input parameters affecting release and transport to ensure most of the radionuclides (e.g., >15 of the 20 currently modeled in groundwater transport calculations) transport through the saturated zone. Input modifications affecting release and transport (e.g., waste package failure, drip shield failure, Kds, conductivities) do not need to be documented for the purpose of these tests since both sets of results being compared will include the same groundwater concentrations and the test is not concerned with the magnitude of those concentrations (merely need to generate groundwater concentration values to use as a starting point for the verification of subsequent calculations). Without modification the base case would only have a small number of radionuclides released to groundwater and forcing the release of additional radionuclides will allow more comprehensive testing of the groundwater protection calculations.

2. Run the modified base case file for a single realization and 10,000 yr simulation period.

3. Obtain the necessary input parameters to calculate groundwater concentrations and radionuclide intakes for a specific time step (e.g., at 10,000 yr) using the spreadsheet. Use the dcagw.ech file (reformatted as dcagw.ech.xls) to obtain radionuclide specific flux to groundwater (ciperallsafromsz in dcagw.f) in Ci/yr, and use tpa.inp file to obtain the input parameters for the annual groundwater pumping volume (ipumpgwp in dcagw.f) in m3, and the drinking water intake in liters/yr. Enter the parameter values in to the spreadsheet (gwprot.handcalc1.r4.xls).

4. Obtain the organ dose coefficients used by the TPA code from the organdf.dat file and enter into the

spreadsheet (gwprot.handcalc1.r4.xls).

5. Compare gross alpha and combined radium concentrations from the spreadsheet with values for the same time step in epa_ave.out file. Agreement within 5% error is sufficient to conclude the values are being calculated correctly by the TPA code.

6. Compare the organ and whole body doses calculated on the spreadsheet with values read for the relevant time step in epa_ave.out file. Agreement within 5% error is sufficient to conclude the values are being calculated correctly by the TPA code.

7. Confirm that the peak doses and concentrations reported in the epapktim.out file match values found in the epa_ave.out file. Because only one realization was executed the "averaged" values for doses and concentrations should be consistent with "peak" values for a given time step. Agreement within 5% error is sufficient to conclude the values are being calculated correctly by the TPA code.

Results/Discussion:

The spreadsheet (gwprot.handcalc1.r4.xls) contains the results of hand calculations and TPA 5.0 beta code output for gross alpha activity, combined radium, and organ and whole body doses. All hand calculated values agree with the TPA code output. Therefore, the conclusion of the testing is that TPA 5.0 beta code groundwater protection calculations for gross alpha activity, combined radium, and organ and whole body doses are being executed and reported in output files (epa_ave.out and epapktim.out) correctly.

An important aspect of ensuring spreadsheet calculations were consistent with the groundwater protection implementation in the TPA code (that is based on 10 CFR Part 63 requirements) involved ensuring the dose calculations included only beta and photon emitting radionuclides as defined by "decay" column in the nuclides.dat data file in the TPA 5.0 beta code. While the individual protection standard based dose calculations include all radionuclides in groundwater, the groundwater protection standards limit the dose calculations to only beta and photon emitters.

Referenced Files:

An attached CD contains the following files.

[Patrick LaPlante, March 27, 2003]

Note: the above test write-up and files listed below was originally written in this notebook then documented in a test plan w/ results and archived files for SCR-327. Because this notebook entry is essentially an early draft of that documentation, please refer to the SCR-327 documentation as the complete record of this test (including archive of files).

tpa.inp

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nuclides.dat
organdf.dat
epa_ave.out
epapktim.out
dcagw.f
dcagw.ech
dcagw.ech.xls
gwprot.handcalc1.r3.xls

[Patrick LaPlante, March 27, 2003]

Correction: The last file in the list above should be named gwprot.handcalc1.r4.xls.

Printed: March 27, 2003

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Entries into Scientific Notebook #170-13E for pages 8 - 10
have been made by **Patrick LaPlante.**

No original text entered into this Scientific Notebook has been removed.

3/27/03.

I have reviewed this scientific notebook and find it in compliance with QAP-001. There is sufficient information regarding methods used for conducting tests, acquiring and analyzing data so that another qualified individual could repeat the activity.

James Winterle 11-9-05