SANDIA REPORT

SAND2012-6333
Unlimited Release
Printed: July 2012

Software Regression Quality Assurance for MACCS2 Version 2.5.0.0 through Version 2.5.0.9

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Abstract

The "State-of-the-Art Consequence Analyses (SOARCA) Project: Uncertainty Analysis" has used a newer version of the MELCOR Accident Consequence Code Systems Version 2 (MACCS2) than what was previously used in the "SOARCA Project Volume 1: Peach Bottom Integrated Analysis," NUREG/CR-7110 Volume 1. A software regression quality assurance program has been implemented for MACCS2. The documentation for the quality assurance from MACCS2 Version 2.5.0.0 through 2.5.0.9 ensures continuity between code versions and provides insight into the changes made within MACCS2.

Acknowledgement

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Acronyms

KI   Potassium iodine
MACCS2   MELCOR Accident Consequence Code System Version 2
QA   Quality assurance
SOARCA   State-of-the Art Reactor Consequence Analyses

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1.0   Introduction

This report outlines the methodology and results from the software regression quality assurance (QA) program for the MELCOR Accident Consequence Code Systems Version 2 (MACCS2) Version 2.5.0.0 through Version 2.5.0.9. This report provides support documentation for the State-of-the Art Reactor Consequence Analyses (SOARCA) project. Specifically the MACCS2 code changes made between the publication of NUREG/CR-7110 Volume 1 [1], and the SOARCA Uncertainty Analysis. This documentation for the QA of MACCS2 Version 2.5.0.0 through Version 2.5.0.9 ensures continuity between code versions and provides insight into the changes made within MACCS2.

2.0 MACCS2 Version 2.5.0.0 to Version 2.5.0.1

Before the software is regression tested and goes through final checkout, all improvements to the code must be tested.

Software Product Name: MACCS2 / WinMACCS

Version Tested Against: MACCS2 v2.5.0.0 / WinMACCS v3.6.2

Version Tested: MACCS2 v2.5.0.1 / WinMACCS v3.6.2

Testing Date: 12/19/2010

Operating System used for Testing:
Windows XP 32 bit, SP3 inside VMWARE Workstation 7.1.3.

Additional Tests and Modifications to Regression Suite:
No changes were required based on this test.

Auxiliary Software Used for Testing:
MS DOS Batch scripts were used to execute regression suite and to move files.

A series of Wolfram Mathematica scripts were used to prepare MS Dos batch files and a summary of differences in tabular form. The Mathematica scripts themselves are not essential to running the regression.

Description of Testing done:
A standard regression test was conducted.

Summary of testing results:
There was a discrepancy between the results for one regression problem. It executed normally under Version 2.5.0 but not Version 2.5.0.1. See the discussion and resolution of this issue in the regression for Version 2.5.0.3 (see Section 4.0). No discrepant results were observed in the other regression testing.

3.0   MACCS2 Version 2.5.0.1 to Version 2.5.0.2

Before the software is regression tested and goes through final checkout, all improvements to the code must be tested.

Software Product Name: MACCS2 / WinMACCS

Version Tested Against: MACCS2 v2.5.0.1 / WinMACCS v3.6.2

Version Tested: MACCS2 v2.5.0.2 / WinMACCS v3.6.2

Testing Date: 02/16/2011

Operating System used for Testing:
Windows XP 32 bit, SP3 inside VMWARE Workstation 7.1.3.

Additional Tests and Modifications to Regression Suite:
No changes were required based on this test.

Auxiliary Software Used for Testing:
MS DOS Batch scripts were used to execute regression suite and to move files.

A series of Wolfram Mathematica scripts were used to prepare MS Dos batch files and a summary of differences in tabular form. The Mathematica scripts themselves are not essential to running the regression.

Description of Testing done:
A standard regression test was conducted. The only differences between Version 2.5.0.1 and Version 2.5.0.2 should be attributable to the use of the new Intel FORTRAN complier.

Summary of testing results:
Of the 55,283 results calculated in the regression set there were a surprising number of discrepancies, as illustrated by Figure 1.
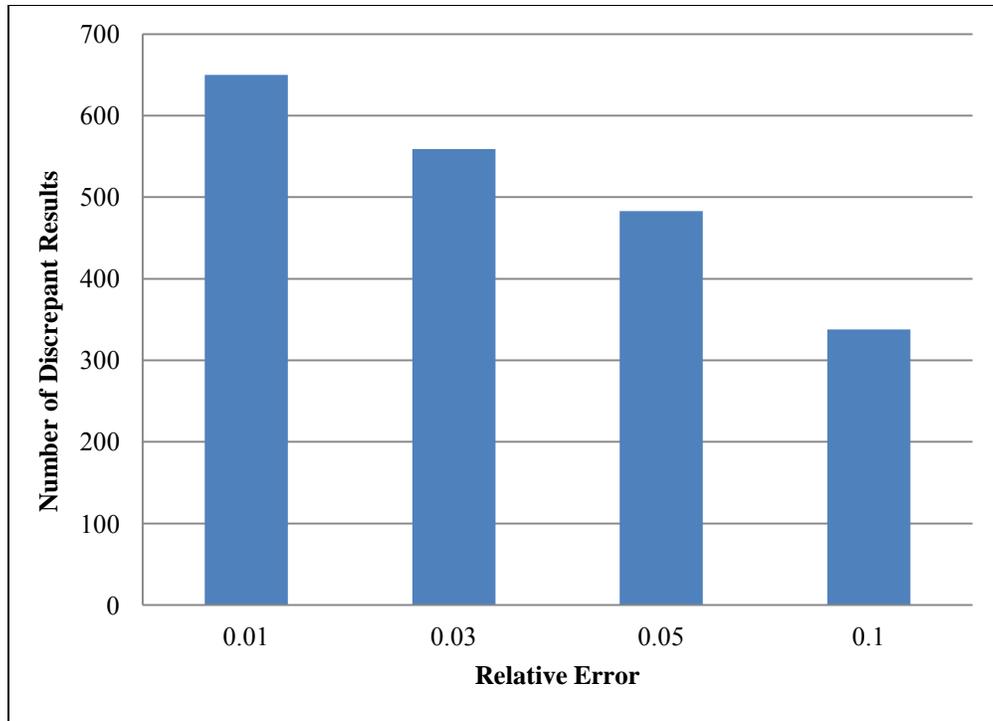
Figure 1: Number of Discrepant Results against the Relative Error

The regression problems with the highest percentages of discrepant results are shown in Table 1.

Table 1: Test Problems with Highest Percentage of Regression Problems

Test Problem	Total Number of Results	Number with Error >0.01
InF_bin	368	328
Multiple_Cohorts_wthreshold2	276	171
Ind_bro	142	17

In each of the three regression problems listed in Table 1, the weather sampling was somewhat different with Version 2.5.0.2 as compared to Version 2.5.0.1.

Inf_bin:
This is an old regression problem that utilizes a weather file and uniform bin sampling of weather.

Multiple_Cohorts_wthreshold2:
This regression problem dates to MACCS2 Version 2.1.0.3. It utilizes a weather file and non-uniform bin sampling.

Ind_bro:
This is an old regression problem. It utilizes a weather file and stratified sampling.

4.0   MACCS2 Version 2.5.0.2 to Version 2.5.0.3

Before the software is regression tested and goes through final checkout, all improvements to the code must be tested.

Software Product Name: MACCS2 / WinMACCS

Version Tested Against: MACCS2 v2.5.0.2 / WinMACCS v3.6.2

Version Tested: MACCS2 v2.5.0.3 / WinMACCS v3.6.2

Testing Dates: 02/16/2011 – 06/28/2011

Operating System used for Testing:
Windows XP 32 bit, SP3 inside VMWARE Workstation 7.1.3.

Additional Tests and Modifications to Regression Suite:
Added the following tests:
- 20Population64DirSUMPOP
- PBSTBO_LNT-20_Cohorts-NoKI-SUMPOP

Replaced the following test:
- Ina_507a with Ina_507aR
  Regression problem „Ina_507a' began to crash starting with Version 2.5.0.1 through Version 2.5.0.3. This regression problem was reviewed by MACCS2 project staff and it was determined to be a poor test problem. The issue with this regression problem is that the array of meteorological dispersion coefficients did not extent far enough to allow virtual source distances to be calculated at all distances of plume travel as atmospheric stability classes changed from time interval to time interval.

  The consensus was that problem „Ina_507a' should be removed from the regression set. In the future it should be replaced in the regression set with problem „Ina_507aR.' The only difference between these two problems is the more extensive array of meteorological dispersion coefficients in the latter problem.

Auxiliary Software Used for Testing:
MS DOS Batch scripts were used to execute regression suite and to move files.

A series of Wolfram Mathematica scripts were used to prepare MS Dos batch files and a summary of differences in tabular form. The Mathematica scripts themselves are not essential to running the regression.

Description of Testing done:

As recommended by the Implementation Plan:

1. Run test cases with the result weighting factor set to SUMPOP against cases with the factor set to PEOPLE. Using two cohorts, create cohort population distributions for the SUMPOP case so that each cohort is 50% of the total PEOPLE population. Set the PEOPLE wtfrac = 0.5 for both cohorts.

2. Run test cases with the result weighting factor set to SUMPOP against cases with the factor set to PEOPLE. Using five cohorts, create cohort population distributions for the SUMPOP case so that each cohort is 20% of the total PEOPLE population. Set the PEOPLE wtfrac = 0.2 for all cohorts.

Both cases should show the overall results as being equal between PEOPLE and SUMPOP.

The following four tests were implemented during regression testing:

Test A:

The technical approach is to devise a matched pair of test problems *(2_Cohort_Test_PeopleX2* and *2_Cohort_Test_SUMPOP)* based on regression test problem „20_Cohort_Test_Alternating.'

The two test problems are intended to provide the same combined cohort result. The following steps were applied:

1. Change to the population in the site file for test problem „2_Cohort_Test_PeopleX2' is twice the population, element-by-element of problem „20_Cohort_Test_Alternating.'

2. Change from 20 cohorts to 2 cohorts and change WTFRAC to 0.5 for each.

3. Make the companion problem, „2_Cohort_Test_SUMPOP.'

4. Edit the site file from „20_Cohort_Test_Alternating' as follows:
   a. Copy the original population array and add it the site file as "population2".
   b. Change 20_Cohort_Test_Alternating to a 2-cohort problem and use the "SUMPOP>Use Existing Site File" WinMACCS2 option.

Run both problems and compare the results for the combined cohort; they should be the same.

Test B:

Prepare the PEOPLE version of a matched pair of test cases. The following steps were applied:

1. Create a new regression problem from „PBSTBO_lnt-6_cohorts-NoKI.'
   a. Save as „PBSTBO_LNT-20_Cohorts-NoKI.'

2. Change from a 6-cohort to a 20-cohort PEOPLE problem by adding another 14 cohorts.
3. Change the original site file by multiplying the population in each grid element by 60.
4. Modify the WTFRAC values to those listed in Table 2.

Table 2: Population Weight Fractions for Test B

Evacuation Cohort	WTFRAC
1	0.016667
2	0.033333
3	0.05
4	0.066667
5	0.083333
6	0.016667
7	0.033333
8	0.05
9	0.066667
10	0.083333
11	0.016667
12	0.033333
13	0.05
14	0.066667
15	0.083333
16	0.016667
17	0.033333
18	0.05
19	0.066667
20	0.083333

5. Prepare the SUMPOP version of this pair of test cases.
6. Create a new regression problem from ‚*lnt-6_cohorts-NoKI.'*
    a. Save as ‚*PBSTBO_LNT-20_Cohorts-NoKI-SUMPOP*.'

7. Change from a six cohort PEOPLE problem to a 20 cohort SUMPOP problem.
8. Change the original site file for the 20 cohorts to those listed in Table 3.

Table 3: 20 Cohort Site File Inputs

Population	Values
1	The original population in regression problem: lnt-6_cohorts-NoKI
2	Two times the original population in regression problem: lnt-6_cohorts-NoKI
3	Three times the original population in regression problem: lnt-6_cohorts-NoKI
4	Four times the original population in regression problem: lnt-6_cohorts-NoKI
5	Five times the original population in regression problem: lnt-6_cohorts-NoKI
6	The original population in regression problem: lnt-6_cohorts-NoKI
7	Two times the original population in regression problem: lnt-6_cohorts-NoKI
8	Three times the original population in regression problem: lnt-6_cohorts-NoKI
9	Four times the original population in regression problem: lnt-6_cohorts-NoKI
10	Five times the original population in regression problem: lnt-6_cohorts-NoKI
11	The original population in regression problem: lnt-6_cohorts-NoKI
12	Two times the original population in regression problem: lnt-6_cohorts-NoKI
13	Three times the original population in regression problem: lnt-6_cohorts-NoKI
14	Four times the original population in regression problem: lnt-6_cohorts-NoKI
15	Five times the original population in regression problem: lnt-6_cohorts-NoKI
16	The original population in regression problem: lnt-6_cohorts-NoKI
17	Two times the original population in regression problem: lnt-6_cohorts-NoKI
18	Three times the original population in regression problem: lnt-6_cohorts-NoKI
19	Four times the original population in regression problem: lnt-6_cohorts-NoKI
20	Five times the original population in regression problem: lnt-6_cohorts-NoKI

Run both problems and compare the results for the combined cohort; they should be the same.

Test C:

To test that WinMACCS Version 3.6.2 correctly partitions the population in a site file the following was done:

- Use test problem „20Population64DirSUMPOP' which uses the ATMOS File from regression problem „20_cohort_test_alternating,' but involves 64 directions instead of 16. The EARLY and CHRONC files are also based on „20_cohort_test_alternating,' but with the following changes:

  o Select the "SUMPOP > Create from existing site file" option.

  o Use a predetermined population distribution, but otherwise the site file was the standard file for the Surry Power Station.

  o Apply data to the WinMACCS "Population Distributions over Cohorts."

  o Apply data to the WinMACCS "Population Distribution Labels."

  o Since this problem used 86 group symbols, apply the array of group symbols by distance and direction in the WinMACCS project.

Run the problem; the "Population1" and "Population 20" values provided in „model 1.out' file should agree with those provided in hand calculations.

Test D:

This test will determine whether SUMPOP runs with one population

Test problems „1_Cohort_Test_People' and „1_Cohort_Test_SUMPOP' are a matched pair of test problems that test whether the SUMPOP option works with only one MACCS2 population. Both problems should execute and give the same results.

Summary of testing results:

Test A: Results are identical for the combined cohort in each of the companion problems.

Test B: Results are identical for the combined cohort in each of the companion problems.

Test C: Calculated MACCS2 populations agree to 5 significant figures or better.

Test D: The SUMPOP option works in the case of only one MACCS2 population.

5.0   MACCS2 Version 2.5.0.3 to Version 2.5.0.4

Before the software is regression tested and goes through final checkout, all improvements to the code must be tested.

Software Product Name: MACCS2 / WinMACCS

Version Tested Against: MACCS2 v2.5.0.3 / WinMACCS v3.6.2

Version Tested: MACCS2 v2.5.0.4 / WinMACCS v3.6.2

Testing Dates: 10/01/2011 – 10/14/2011

Operating System used for Testing:
Windows XP 32 bit, SP3 inside VMWARE Workstation 7.1.3.

Additional Tests and Modifications to Regression Suite:
No changes were required based on this test.

Auxiliary Software Used for Testing:
MS DOS Batch scripts were used to execute regression suite and to move files.

A series of Wolfram Mathematica scripts were used to prepare MS Dos batch files and a summary of differences in tabular form. The Mathematica scripts themselves are not essential to running the regression.

Description of Testing done:
MACCS2 Bug 769:
Three regression problems that involved the potassium iodine (KI) model showed a significant number of unanticipated differences between Version 2.4.0.6 and Version 2.5.0.3. The error causing the unanticipated differences was fixed in Version 2.5.0.4.

The regression set was run informally using MACCS2 Version 2.5.0.4 and compared against Version 2.5.0.3. There were result differences in only three test projects: ina_n_bug201_238, ina_n_fgr13_KI_model, and KI-Modl+-+.

The Version 2.5.0.4 results for these three projects are essentially identical with the results that were obtained using Version 2.4.0.6. There were small differences in the peak probability, peak result, and higher percentiles of some result distributions.

MACCS2 Bug 789:
Warning messages of the type shown below were being printed to the MACCS2 status file.

Warning: Bounds of dispersion sigma-z lookup table exceeded for the following stability classes: class 4, class 5, class 6

According to the software implementation plan, changes were made to Version 2.5.0.4 that were intended to prevent any warnings from being written to the Model*MaxStat.log file.

Testing for correction of this bug involved running regression problem "Ina_507a" under Version 2.5.0.3 to verify that the bug is exhibited, and under Version 2.5.0.4 to confirm that the bug is no longer logged to the Model*MaxStat.log file. This test was executed using WinMACCS 3.6.3. Results are archived at:

This test confirms that MACCS2 Bug 789 was not fixed in a comprehensive way. The Model*MaxStat.log files created under Versions 2.5.0.3 and Version 2.5.0.4 both log files contain warning messages.

Summary of testing results:
MACCS2 Bug 769:
It was expected that the only the three projects identified above would exhibit changes relative to Version 2.5.0.3. It was expected that correcting MACCS2 Bug 769 would cause the results for the three effected projects under Version 2.5.0.4 to closely agree with the results observed under Version 2.4.0.6, since the bug was apparently introduced with Version 2.5.0.0.

Small differences in Version 2.5.0.4 relative to Version 2.4.0.6 results in values of peak probability, peak result, and higher percentiles of some result distributions are apt to be due to minor differences in weather sampling and number rounding. These types of differences have been seen before and appear be related to the recent change in compilers (see Section 3.0).

MACCS2 Bug 789:
The bug still can be observed with regression problem "Ina_507a" when executed under WinMACCS Version 3.6.3 with MACCS2 Version 2.5.0.4.

6.0   MACCS2 Version 2.5.0.5

This version of MACCS2 is an intermediate version. It was neither regression tested nor was a QA assessment applied. This version was created in January 2012 and was subsequently replaced by MACCS2 Version 2.5.0.6 in February 2012.

7.0 MACCS2 Version 2.5.0.4 to Version 2.5.0.6

Before the software is regression tested and goes through final checkout, all improvements to the code must be tested. Version 2.5.0.6 was not fully regression tested. It was developed in conjunction with Version 2.5.0.7 discussed in Section 8.

Software Product Name:　　　　　　MACCS2 / WinMACCS

Version Tested Against:　　　　　　MACCS2 v2.5.0.4 / WinMACCS v3.6.3

Version Tested:　　　　　　　　　　MACCS2 v2.5.0.6 / WinMACCS v3.6.3

Testing Dates:　　　　　　　　　　04/28/2012 – 05/02/2012

Operating System used for Testing:
Windows XP 32 bit, SP3 inside VMWARE Workstation 7.1.3.

Additional Tests and Modifications to Regression Suite:
Add problem "DenMOD1b_921 and retire problem "DenMOD1b."

Description of Testing done:
MACCS2 Bug 747: Error in type C and type D output.
The testing of behavior with respect to „old decks' was not required. „Old decks' would be those where FRACLD was defined in CHRONC, if not defined in the site file. WinMACCS Version 3.6.3 places FRACLD in the EARLY deck if not defined in the site file. Testing performed and results are listed in Table 4.

Table 4: MACCS2 Bug 747 Testing and Results

Description	Testing Performed and Result

The type C and type D output shows zero doses regardless of the threshold value (ELEVDOSE) specified, although the print flag appears to be working correctly (i.e., Doses are printed out for all grid elements, when the print flag is set to true. The land area exceeding the dose threshold and/or exceeding concentration reports a value of zero).
 	
Case:
   CHRONC excluded,
   Site File included.
	Build problem ‚Ina_n747B' by copying ‚Ina_n,' importing cards identified in the footnote[1]. However, unselect CHRONC module.
	
	Problem executed successfully in Version 2.5.0.4 but gives zero for land area exceeding dose or concentration thresholds.
	
	Problem executes successfully in Version 2.5.0.6 and gives non-zero values for land area exceeding dose or concentration thresholds.

If running an old MACCS2 input deck and not running CHRONC, and not using a site data file and requesting C and D output, no error will be reported because the results will be wrong.
 	
Case:
   CHRONC excluded,
   Site File excluded.
	Make problem ‚Ina_n747C' like ‚Ina_n747B.' Unselect CHRONC, and remove site file.
	
	During creation of this project, WinMACCS Version 3.6.3 recognizes that FRACLD is required and considers the value as early input.
	
	For Version 2.5.0.4, the problem executes but erroneous zero results are reported as expected. For Version 2.5.0.6, the problem executes and non-zero results are reported in the output file where expected.

If running an old MACCS2 input deck and running CHRONC and requesting C and D output, the calculation will proceed normally. In this case, FRACLD will be read from the CHRONC input file and used if not using a site data file.
 	
Case:
   CHRONC included,
   Site File excluded.
	Make problem ‚Ina_n747D' in the same fashion as ‚Ina_n747B.' Keep CHRONC active and remove site file.
	
	FRACLD had to be entered via the Early variable menu of WinMACCS. Regional characteristics form has to be completed through the CHRONC menu.
	
	For Version 2.5.0.6, the non-zero results are reported in the output file where expected. As expected, Version 2.5.0.6 was able to find FRACLD in this case.

---

[1]Imported cards:
```
 TYPECNUMBER          2
TYPECOUT001  L-EDEWBODY  0.01      .FALSE.
TYPECOUT002  L-EDEWBODY  0.1       .TRUE.
TYPEDNUMBER          2
TYPEDOUT001  1         Cs-137  10000.  .TRUE.
TYPEDOUT002  13        Sr-90   10000.  .FALSE.
```

Table 4: MACCS2 Bug 747 Testing and Results (continued)

Description	Testing Performed and Result

If running an old MACCS2 input deck and running CHRONC and requesting C and D output, the calculation will proceed normally. In this case, FRACLD will be read from the CHRONC input file and used if not using a site data file.
 	
Case:
   CHRONC included,
   Site File excluded.
	Make a problem in the same fashion as 'Ina_n247D,' and name it 'Ina_n247E.' Execute through WinMACCS Version 3.6.3 using MACCS2 Version 2.5.0.4.
	
	FRACLD had to be entered via the Early variable menu of WinMACCS. Regional characteristics form has to be completed through the CHRONC menu.
	
	For Version 2.5.0.4, the problem produced the following error message:
	
	                >>>>>INPUT ERROR>>>>>
	   >>>>>CALLED FROM SUBROUTINE INCHRN, LOOKING
	           FOR FRACLD AT RECORD: CHFRACLD001
	             >>>>>RECORD ID NOT LOCATED
	   !!! ERROR--FORCING ABNORMAL EXIT !!! INCHRN.
	
	As expected, Version 2.5.0.4 could not locate FRACLD in the problem.

MACCS2 Bug 783: DCF path too long to process error message from MACCS2.
An error was reported by a MACCS2 user when using DCF file name/path:

C:\Users\ymcclel\Documents\Department6762Folders\SOARCA-Files\JapanFiles\Practice-FUKUSHIMA-1Plant\Data\FGR13GyEquivDCF.INP

Steps proposed for testing:
1. Create a file path at least as long as the file path given above (i.e., 123 characters long), with the DATA directory being eight directories down from the root directory.

2. The bug is reported to have been fixed in Version 2.5.0.6.

3. Verify that the bug is observed through WinMACCS Version 3.6.3 in MACCS2 Version 2.5.0.4.

4. Verify that the bug does not appear in MACCS2 Version 2.5.0.6.

Implementation:
Created a MACCS2 project from regression project 'IND_ju1.mxd.' Placed the project in the following file folder:

C:\M2\BugEnh\2.5.0.6+3.6.3\InD_ju1__783_01234567890123456789012345678901234567890123456789\Depth5\Depth6\Depth7\InD_ju1.mxd

The problem used a DCF file located in the following file folder:

C:\M2\BugEnh\2.5.0.6+3.6.3\InD_ju1__783_
012345678901234567890123456789012345678901234567889\Depth5\Depth6\Depth7\Data\Dos
d825_012345678901234567890123456789.inp

Test Results:
The test problem executed successfully both under Version 2.5.0.4 and Version 2.5.0.6.
Therefore MACCS2 Bug 783 is resolved. SNL was unable to demonstrate that the bug occurs in
Version 2.5.0.4. In what version it was resolved was not investigated.

MACCS2 Bug 802: Discrepant result in constant weather problem (ina_n_bug245-A) with new
                            Intel compiler.

This was the constant weather regression problem with the greatest prevalence of logged
differences reported by the BinCompare.exe utility for the new and old compiler (e.g. MACCS2
Version 2.5.0.2 vs Version 2.5.0.1). There were differences in early fatality distance and in the
ERL Fat/Total results.

Based on the analysis of the error provided by the programme, there is reason to believe that the
early fatality distance and the ERL Fat/Total results obtained for this problem with
Version 2.5.0.6 should agree rather closely with those obtained with Version 2.5.0.1 despite the
compiler differences. This particular test problem is non-stochastic; it does not depend on
weather sampling or on random number sequences.

Proposed test plan:
Run regression problem „ina_n_bug245-A' under Version 2.5.0.6 and compare to the results
with Version 2.5.0.1.

Test Results:
The results for the early fatality distance and in the ERL Fat/Total results obtained for this
problem with Version 2.5.0.6 agree exactly with those obtained with Version 2.5.0.1. A minor
discrepancy was observed in the result for ERL INJ/SKIN ERYTHEMA health effects cases,
changing from 0.0955 under Version 2.5.0.1 to 0.0935 under Version 2.5.0.6.

MACCS2 Bug 921: The lower limit of the input variable PLMDEN needed to be lowered.
The MACCS2 programmer reported that lower limit for the variable PLMDEN was changed
from 0.2 to 0.02. This is consistent with WinMACCS and the MACCS2 User Manual [2, 5].

Proposed test plan:
Take regression problem „DenMod1b;' change PLMDEN to 0.02 and 5.0 for the first and second
plumes, respectively; save as project „DenMod1b_921.' These parameter values were chosen to
verify both the upper limits and lower limits are accepted. Verify that the project executes
without generating errors.

Test Results:

It executed without the complaint that was attributable to the changes made. However, the „model1.out' file includes an error message related to output type 10. Note that this is essentially regression problem „DenMod1b' with changes to PLMDEN only, and that problem previously executed without writing error messages into „model1.out' under Version 2.5.0.4. This behavior was logged into Melzilla as MACCS2 Bug 963.

Summary of testing results:

1. <u>MACCS2 Bug 747</u>: Error in type C and type D output.
   The tests did not verify „old deck' behavior. Test results are as expected given the description provided in the Software Implementation QA Form.

2. <u>MACCS2 Bug 783</u>: DCF path too long to process error message from MACCS2.
   The test problem executed successfully under Version 2.5.0.6; bug 783 is resolved.

3. <u>MACCS2 Bug 802</u>: Discrepant result in constant weather problem (ina_n_bug245-A) with new Intel compiler.

   Early fatality distance and in the ERL Fat/Total results obtained for this problem with Version 2.5.0.6 now agrees exactly with those obtained with Version 2.5.0.1., as expected. A minor discrepancy was observed in the result for ERL INJ/SKIN ERYTHEMA health effects cases, changing from 0.0955 under Version 2.5.0.1 to 0.0935 under Version 2.5.0.6, (~2%) difference; this was noted but not investigated or logged as an error.

4. <u>MACCS2 Bug 921</u>: The lower limit of the input variable PLMDEN needed to be lowered.
   It executed without complaint that was attributable to the changes made. However, the „model1.out' file includes an error message related to output type 10. This unexpected behavior was logged into Melzilla as MACCS2 Bug 963, but was not investigated by the software tester.

8.0   MACCS2 Version 2.5.0.4 to Version 2.5.0.7

Before the software is regression tested and goes through final checkout, all improvements to the code must be tested. Version 2.5.0.7 was developed during the same time as Version 2.5.0.6 and all changes discussed in Section 7 were incorporated into Version 2.5.0.7.

Software Product Name: MACCS2 / WinMACCS

Version Tested Against: MACCS2 v2.5.0.4 / WinMACCS v3.6.3

Version Tested: MACCS2 v2.5.0.7 / WinMACCS v3.6.3

Testing Date: 04/28/2012 – 05/02/2012

Operating System used for Testing:
Windows XP 32 bit, SP3 inside VMWARE Workstation 7.1.3.

Additional Tests and Modifications to Regression Suite:
No changes were required based on this test.

Auxiliary Software Used for Testing:
MS DOS Batch scripts were used to execute regression suite and to move files.

A series of Wolfram Mathematica scripts were used to prepare MS Dos batch files and a summary of differences in tabular form. The Mathematica scripts themselves are not essential to running the regression.

Description of Testing done:
A standard regression test was conducted.

Description of Testing done:
MACCS2 Bug 885:
Plume Meander Model shown in the U.S. Nuclear Regulatory Commission's Regulatory Guide 1.145 [6] was originally implemented incorrectly. Values should have been interpolated using a logarithmic scale not a normal scale. The solution implemented was to replace the following equation in the FSGY and FSGYIN functions:

$$f(u) = 1 - (u-u1)/(u2-u1) * (m-1)/m$$
$$when: \ u1 < u < u2$$

with

$$f(u) = (1/m) * exp(\ log(m) - ((log(u)-log(u1))/(log(u2)-log(u1))) * log(m) \ )$$
$$when: \ u1 < u < u2$$

Proposed testing:

Depending on airspeed out to the transition distance (default 800 meter) the model calculates f(u) by one of three equations. This update is expected to affect only one of these three equations, with the computational change described above.

A. Verify that when the initial wind speed < u1, the plume meander model option provides the same result with Version 2.5.0.7 as with Version 2.5.0.4, the last regression tested version.

B. Verify that when the initial wind speed > u2, the plume meander model option provides the same result with Version 2.5.0.7 as with Version 2.5.0.4, the last regression tested version.

C. Verify that when the initial wind speed is intermediate, u1 > wind speed > u2, the plume meander model option provides different results with Version 2.5.0.7 as compared with Version 2.5.0.4, the last regression tested version.

Summary of testing results:

Test A: The results with the two MACCS2 versions agree exactly.

Test B: The results with the two MACCS2 versions agree exactly.

Test C: There are small differences in the results for the first plume as expected, although the differences in σ_y are a few meters at any distance. The differences that are observed are in the same direction as those calculated independently.

9.0 MACCS2 Version 2.5.0.8

This version of MACCS2 is an intermediate version. It was neither regression tested nor was a QA assessment applied. This version was created in early May 2012 and was subsequently replaced by MACCS2 Version 2.5.0.9 in late May 2012.

10.0 MACCS2 Version 2.5.0.7 to Version 2.5.0.9

Before the software is regression tested and goes through final checkout, all improvements to the code must be tested.

Software Product Name: MACCS2 / WinMACCS

Version Tested Against: MACCS2 v2.5.0.7 / WinMACCS v3.6.3

Version Tested: MACCS2 v2.5.0.9 / WinMACCS v3.6.3

Testing Date: 05/17/2012 – 05/30/2012

Operating System used for Testing:
Windows XP 32 bit, SP3 inside VMWARE Workstation 7.1.3.

Additional Tests and Modifications to Regression Suite:
No changes were required based on this test.

Auxiliary Software Used for Testing:
MS DOS Batch scripts were used to execute regression suite and to move files.

A series of Wolfram Mathematica scripts were used to prepare MS Dos batch files and a summary of differences in tabular form. The Mathematica scripts themselves are not essential to running the regression.

Description of Testing done:
MACCS2 Bug 963: Unexpected error message appears concerning Type 10 output.

> *>>>>>INPUT ERROR>>>>>*
> *>>>>>CALLED FROM SUBROUTINE IXOT10, LOOKING FOR PRINT_FLAG_10 AT*
> *RECORD: TYP10OUT001*
> *>>>>>LOGICAL VALUE NOT FOUND*

Implemented a solution as follows:
Reading of Logical flags were not originally implemented to be an optional value on a card. Reading of Logical flags on a card have now been implemented to be optional by using the OPTCARD variable in the code. The print flag portion of the Result Type 10 input card will no longer cause an input error message to be printed to the output file if the ".true." or ".false." print string is not included on the input card.

Proposed method of testing:
This bug was first recognized under Version 2.5.0.6 with test problem DenMod1b_921. When the same problem is run with Version 2.5.0.9 no error message should appear in the model1.out file.

MACCS2 Bug 966: Change wording of error message when the σ_y lookup table has been exceeded.

Use the word "ERROR" instead of "WARNING," since this is a program stop condition.

Implemented a solution as follows:
Reword the error message to use the word "ERROR" instead of "WARNING." The error message now reads as follows:

> *ERROR: The Dispersion SIGMA Y Lookup table has been exceeded.*
> *The sigma-y lookup table exceeded for stability class 6.*
> *Current Sigma Y Distance value = 7561.956*
> *Maximum Sigma Y Table value = 4424.800.*
> *!!! ERROR--FORCING ABNORMAL EXIT !!!*
> *FSGYIN: EXCEEDED RANGE OF SIGMA_Y LOOKUP TABLE*

Proposed method of testing:
This issue was first recognized in test problem Ina_507a under Version 2.5.0.4. If this same problem is executed under Version 2.5.0.9, then the result should provide the error message described above.

Summary of testing results:
MACCS2 Bug 963: The error message no longer occurs.

MACCS2 Bug 966: The error message now appears as described above.

11.0 References

1. Sandia National Laboratories, "State-of-the-Art Reactor Consequence Analyses Project Volume 1: Peach Bottom Integrated Analysis," NUREG/CR-7110 Volume 1, Nuclear Regulatory Commission, Washington DC: January 2012

2. Chanin, D.I., and M.L. Young, "Code Manual for MACCS2: Volume 1, User's Guide," NUREG/CR-6613 Volume 1, Nuclear Regulatory Commission, Washington DC: May 1998.

3. Chanin, D.I., and M.L. Young, "Code Manual for MACCS2: Volume 2, Preprocessor Codes COMIDA2, FGRDCF, IDCF2," NUREG/CR-6613 Volume 2, Nuclear Regulatory Commission, Washington DC: May 1998.

4. Jow, H.N., et al., "MELCOR Accident Consequence Code System (MACCS) Model Description," NUREG/CR-4691 Volume 2, Nuclear Regulatory Commission, Washington DC: February 1990.

5. McFadden, K.L., et. al., "WinMACCS, a MACCS2 Interface for Calculating Health and Economic Consequences from Accidental Release of Radioactive Materials into the Atmosphere – User's Guide and Reference Manual, WinMACCS Version 3 – DRAFT," Draft NUREG/CR, Nuclear Regulatory Commission, Washington DC: Draft Manuscript Completed – July 2007.

6. U.S. Nuclear Regulatory Commission, "Atmospheric Dispersion Models for Potential Accident Consequence Assessments at Nuclear Power Plants," Regulatory Guide 1.145 Revision 1, Washington DC: November 1982.

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