



Software Quality Assurance

ERRORS IN MACCS2 χ/Q CALCULATIONS

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PURPOSE

This Advisory provides information on software quality assurance problems related to the use of MACCS2 versions 1.13.1 and 2.4 to determine atmospheric dispersion factors (χ/Q s).

BACKGROUND

The Hanford Waste Treatment Plant (WTP) project used the MACCS2 code to generate χ/Q s for use in the updated accident consequence analyses. Version 2.4 is the latest version of MACCS2 and the only version currently supported by the code developer Sandia National Laboratories (SNL) that developed the code for the Nuclear Regulatory Commission. WTP nuclear safety personnel prepared the required software life cycle documentation and independently validated and verified MACCS2 version 2.4 for use on the project.

When χ/Q calculations using MACCS2 versions 2.4, and 1.13.1 were compared, the results varied by less than 30%. This is not unexpected since version 2.4 was upgraded to include several improvements in the atmospheric dispersion models. Further investigation revealed that erroneous calculations of undepleted and depleted χ/Q s were being generated when the user provided insufficient information in lookup tables for sigma-y and sigma-z. The major impact was observed for mean values. Additionally, a problem related to inconsistent results for sigma-z values for depleted χ/Q s was noted in the output at a distance from the source.

PROBLEM WITH χ/Q CALCULATIONS

The problem noted by WTP is described as follows:

- The user created a lookup table for the lateral and vertical dispersion coefficients, sigma-y and sigma-z.
- The table did not extend to sufficiently long distances for all possible weather patterns that occurred during the meteorological data sampling process.
- Problems occurred for a few weather trials when stability class changed to a more stable condition during the calculation and the virtual source location was large.
- The code tried to use data beyond the final distance listed in the lookup table. The result was erroneous and sometimes negative values for sigma-z. This resulted in unrealistic values of χ/Q and other derived quantities.
- The code did not issue a warning message or stop execution; instead, it continued calculating and produced erroneous results.

The following approaches have been identified for avoiding the problems noted above:

1. For the lookup table issue with sigma-y and sigma-z, increase the distance in the lookup table to values well beyond the distances of interest; however, if lookup tables are not used, this is not an issue. Both versions 1.13.1 and 2.4 are affected.
2. For the inconsistent sigma-z printed values for depleted χ/Q issue, turn off the DAY_NIGHT mixing height option when using version 2.4. This is only a problem with version 2.4 and does not exist with version 1.13.1.

CONCLUSIONS

The following simple check can be used to determine if there is a problem with user's MACCS2 lookup tables:

- Set IDEBUG to 3
- Rerun the calculation with the same choice of weather sampling that is being used in the analyses.
- Scroll down through the output file and look for data for the first weather trial, which will begin with "BEFORE ADJUSTMENT, SELECTED..."
- Search for occurrences of the character string "-", (i.e., a space followed by a minus sign).

If MACCS2 attempts to go beyond the last value in the lookup table, PLSIGZ goes negative. As a result, values of GL AIRCON, GRNCON, and GL χ/Q also go negative. If negative values of these variables are seen in the output file, the lookup tables need to be extended to longer distances. This check needs to be performed once for each combination of weather file, weather sampling strategy, and lookup table.

As a result, the following actions are being taken by SNL:

- Known MACCS2 users have been notified of the problem.
- The next release of MACCS2 will contain a check for this problem and terminate with an error message if it occurs.
- A high priority will be given to developing an on-line error reporting system that will facilitate communication of any problems encountered by users.

ADDITIONAL SOURCES OF INFORMATION

WTP analysis is given in a paper "Validity of Using MACCS2 Computer Program to Determine Atmospheric Dispersion Factors for Use in WTP Safety Analysis." For copies, contact Roger Lanning at rdlannin@becthel.com. For questions regarding the MACCS2 problem, contact Nathan Bixler at nbixler@sandia.gov. Other questions should be directed to Subir Sen at subir.sen@hq.doe.gov.

Glenn S. Podonsky
Chief Health, Safety and Security Officer
Office of Health, Safety and Security