CMAS has received its first development version of **CMAQ-MADRID** from AER, consisting of the source code, documentation, and benchmark datasets for 3 examples of CMAQ-MADRID applied to the SCAQS 1987 episode, for release to the public. The code was developed by AER under an EPRI contract using CMAQ Version 4.2.1 (released by EPA in July 2002) as the starting point. The benchmark cases exercised a combination of options using either MADRID1 or MADRID2, for the treatment of particle growth, and one of two different representations, using either 8 sections or 2 sections for the particle size distribution. They also used three different combinations of compiler and processor as described below. CMAS staff attempted to compile and rerun all 3 examples on a Beowulf Cluster running RedHat Linux Version 7.3. Results of these tests, documented below, show that the choice of the processor, the compiler version, and the number of aerosol size sections all have impacts to varying degrees on the reproducibility of the benchmark results.

Example 1: **(MADRID1 with 8 sections)**

Run A1: AER used Portland Group Compiler Version 4 (PG4) and AMD 2100+ processor
Run C1: CMAS used PG5 and AMD Athlon 1.6 GHz processor
Run C2: CMAS used PG5 and Intel Xeon 2.4 GHz processor
Run C3: CMAS used PG5 and Intel Xeon 2.8 GHz processor
Run C4: CMAS used PG4 and AMD Athlon 1.6 GHz processor

To evaluate the extent of differences between the CMAS simulation results and those of AER, we calculated the percentage of model grid cells that had a maximum absolute difference of 5 %. The comparisons of model outputs from the C1-C4 runs with A1 are shown for all modeled species in the "MADRID_Eg1" worksheet of the Excel file included in the documentation. The time and location of the maximum difference (C1 versus A1) for each species during the simulation period are also shown. While the gas-phase species were reproduced almost exactly (with less than 1 % of the grid cells with absolute differences greater than 1.0E-6), many of the PM species had large differences in CMAS runs C1 to C3. To cite a few examples, SO_4 and EC showed a relative difference of more than 5 % in many sections of the size distributions in about 40-50 % of the grid cells; NO_3 showed similar differences in 10-30 % of the grid cells. The outputs from runs C2 and C3 were identical, thus eliminating the possibility of any effects due to a change in the processor speed.

Since the CMAS runs C1 to C3 did not quite match the outputs from A1, we used PG4 in our processing in Run C4. The outputs from Runs A1 and C4 were identical.

Example 2: (MADRID2 with 2 sections)

Run A2: AER used PG4 and AMD 2100+ processor
Run C6: CMAS used PG5 and AMD Athlon 1.6 GHz processor
Run C7: CMAS used PG5 and Intel Xeon 2.8 GHz processor
Run C8: CMAS used PG4 and AMD Athlon 1.6 GHz processor

Similar analyses to those of Example 1 were done with Example 2 outputs, as shown in the "MADRID_Eg2" worksheet of the Excel file. For this example, while some of the gas phase species from runs C6, C7 and C8 had identical outputs compared to A2, many of the PM species differed in up to 2 % of the total grid cells by more than 5 %. Also, the outputs from A2 matched those of C6 and C8 slightly better than C7, probably due to the fact that A2 and C6 were run on the same processor. It should be noted that, unlike the case of Example 1, none of the CMAS runs showed identical results for the PM species compared to Run A2, even with the same versions of the compiler and processor. There were no consistent patterns (either spatially or temporally) with these differences These differences need further investigation in light of their magnitudes for PM species in some locations.

Example 3: (MADRID1 with 2 sections)

Run A3: AER used PG3 and Intel 2.2 GHz processor
Run A4: AER used PG4 and Intel 2.2 GHz processor
Run C9: CMAS used PG4 and AMD Athlon 1.6 GHz processor
Run C10: CMAS used PG4 and Intel Xeon 2.4 GHz processor

Since the runs A4 and C10 for example 3 used identical versions of compilers and processors (PG4 and Intel), we were able to successfully reproduce AER's benchmark results. Comparisons are shown in the "MADRID_Eg3" worksheet. The outputs from C9 differed only slightly from those of C10, showing that in this example, the processor difference did not matter significantly.

To conclude, CMAS was successful in reproducing most of the benchmark results of all three examples provided by AER. When identical versions of compiler and processors were used, examples 1 and 3 (MADRID1) were reproduced exactly, whereas example 2 (MADRID2) had relative differences of more than 5 % in up to 2 % of the total grid-cells. Further, our results for example 1 (i.e., MADRID1 with 8 sections) from Runs C1-C3 showed larger-than-acceptable differences from the benchmark results showing that MADRID1 is significantly more sensitive than MADRID2 to the compiler version as well as the processor. It is possible that this is because MADRID1 uses a greater number of size sections, and is thus numerically more intensive than MADRID2.

The CMAQ-MADRID source code, documentation and build and run scripts for the 3 example cases are available for download from the **CMAS Model Clearinghouse (http://www.cmascenter.org/modelclear.shtml)**. The input and output files, however, are not included in the Clearinghouse due to their large size, and are available upon request from CMAS.

Questions or comments about CMAQ-MADRID should be directed to Krish Vijayaraghavan at AER (krish@aer.com). Questions or comments about the results of the CMAS testing, and requests for the benchmark datasets may be directed to either of the CMAS software development coordinators, Sarav Arunachalam and Uma Shankar (sarav@unc.edu; ushankar@unc.edu).