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WHAT'S NEW IN MCIP2?

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1. INTRODUCTION

The Community Multiscale Air Quality Model's (CMAQ's) Meteorology-Chemistry Interface Processor (MCIP2) has been updated for release from the Community Modeling and Analysis System (CMAS) Center. Several changes have been included in the new release, MCIP Version 2.3, ranging from new capabilities to minor bug fixes. The full suite of changes is described below. Users should refer to the "CHANGES" file in the MCIP2 release to find out which routines are impacted by each change to MCIP2.

2. CHANGES IN MCIPv2.3

The following code changes were introduced into MCIP2. Each change is documented with a rationale for the change, the impact of the change, and, where applicable, credit for identifying or resolving the issue.

Added processing of the hydrometeor field, graupel.

Rationale: Three advanced microphysics options that generate prognostic graupel are available in MM5. MCIP2 should pass that field on to CMAQ, if the field is available. Previous releases of MCIP2 will run and ignore graupel if it is in MM5 output. In that case, however, a portion of the hydrometeor mixing ratio is not considered by CMAQ.

Impact: One field (QG) has been added to METCRO3D, if it is available in MM5, increasing MCIP2 output file size.

Credits: Donna Schwede (U.S. EPA ORD, Research Triangle Park, NC) made the initial code changes to include graupel in MCIP2, and Rob Gilliam (U.S. EPA ORD, Research Triangle Park, NC) assisted with initial testing.

Added a work-around for an NCAR bug in processing vegetation fraction for the Pleim-Xiu land-surface model in MM5.

Rationale: NCAR introduced a code change in MM5v3.5 (which was later corrected in MM5v3.6.2) that inadvertently changed the vegetation fraction (VEGFRC) in the Pleim-Xiu land-surface model to an unrealistic (i.e., two orders of magnitude too large) value every 24th hour in the MM5 simulation following MM5 initialization. When MCIP2 used the unrealistic VEGFRC values, negative dry deposition velocities could occur on one hour each day. These dry deposition velocities were generally detected only if they were severe enough to cause CMAQ to crash.

Impact: The risk of negative dry deposition velocities from this NCAR bug in MM5 has been mitigated. The previous hour's vegetation fraction is used in MCIP at times when unrealistic VEGFRC values are detected, leading to minor differences in dry deposition velocities from what would have been ordinarily calculated by the Pleim-Xiu land-surface model if MM5 did not have the bug. Note that this correction will not work if MM5 and CMAQ are initialized at the same hour (i.e., no "spin-up" time allowed for MM5, or a 24-h "spin-up" time allowed).

Credits: Donna Schwede (U.S. EPA, Research Triangle Park, NC) made the initial code changes in MCIP2. Brian Timin (U.S. EPA OAQPS, Research Triangle Park, NC), Bret Anderson (U.S. EPA Region 7, Kansas City, KS), and Andy Hawkins (Kansas Department of Health and Environment, Topeka, KS) brought this issue to our attention.

Corrected I/O API header settings for the polar stereographic and Mercator projections.

Rationale: The I/O API header variables for the Mercator and polar stereographic projections were incorrect.

Impact: MCIP2 output can be used properly by SMOKE and visualized in PAVE in these projections.

Credits: Maria Prodanova-Boiadjieva (National Institute of Meteorology and Hydrology, Sofia, Bulgaria), Éric Giroux (National Research Council Canada, Ottawa, ON, Canada), and Narisara Thongboonchoo (Univ. of Iowa, Iowa City, IA) brought this issue to our attention. Luca Delle Monache (Univ. of British Columbia, Vancouver, BC, Canada) provided a test data set to help resolve this issue. Discussions with Carlie Coats (Baron Advanced Meteorological Systems, Research Triangle Park, NC) and Todd Plessel (Lockheed Martin, Research Triangle Park, NC) also contributed to the proper resolution of this issue.

Added a minimum PBL height for MM5 simulations with the Mellor-Yamada (Eta) PBL scheme.

Rationale: The PBL height algorithm in the Mellor-Yamada (Eta) PBL scheme in MM5 sometimes produces negative PBL heights. These values can lead to negative WSTAR values that can cause CMAQ to crash.

Impact: A minimum PBL height of lowest model full layer was set for MM5 runs with the Eta PBL scheme to

prevent very small and negative PBL heights from being used by SMOKE and CMAQ.

Credits: Shaheen Tonse (Lawrence Berkeley National Laboratory, Berkeley, CA) and Jinyou Liang (Bay Area Air Quality Management District, San Francisco, CA) brought this issue to our attention.

Corrected minor formatting bugs in GRIDDESC file.

Rationale: The format of the GRIDDESC file output from MCIP was not compatible with other CMAQ programs.

Impact: Users can read the MCIP2-generated GRIDDESC file in SMOKE, CMAQ, and other programs.

Credits: Jeff Stehr (Univ. of Maryland, College Park, MD) and Rafik Djouad (SENES, Richmond Hill, ON, Canada) brought this issue to our attention.

Modified output routines so that the hydrometeor species and Pleim-Xiu arrays are only written to output if options in MM5 generate those fields.

Rationale: It wastes disk space to output arrays that are entirely filled with "missing" values.

Impact: Results in smaller METCRO3D files when less-sophisticated microphysics options are used in MM5. Also, results in smaller METCRO2D files when Pleim-Xiu land-surface model is not used in MM5.

Restored the GRIDBDY2D file to MCIP2 output.

Rationale: GRIDBDY2D has no downstream processor in the CMAQ system that uses this file. However, GRIDBDY2D contains the latitude and longitude coordinates of the CMAQ boundary cells, and this information is handy for initializing CMAQ from fields from another (e.g., global) model.

Impact: An additional, but very small file is created in MCIP2 output.

Credits: Rohit Mathur (U.S. EPA ORD, Research Triangle Park, NC) and Maria Prodanova-Boiadjieva (National Institute of Meteorology and Hydrology, Sofia, Bulgaria) demonstrated the utility of this file.

Restored the full-level Jacobian to output.

Rationale: The full-level Jacobian is required as part of a correction in the vertical diffusion algorithm in CMAQ.

Impact: One output field (JACOBS) is added to METCRO2D and one output field is added to METCRO3D (JACOBF), increasing MCIP2 file sizes.

Credits: Jeff Young (U.S. EPA ORD, Research Triangle Park, NC) identified the need for the full-level Jacobian.

Refined error-checking that prevents users from defining thinner top and/or bottom layers than are available in MM5 output.

Rationale: The error-checking in statflds.F was not robust, and it occasionally resulted in MCIP2 stopping unnecessarily (due to real-number comparison and machine precision issues).

Impact: Users who are properly setting a vertical structure in MCIP2 should not be unnecessarily stopped in MCIP2.

Credits: Several users have identified this problem, including Alexis Zubrow (Univ. of Chicago, Chicago, IL), Aijun Xiu (Carolina Environmental Program, Chapel Hill, NC), Santosh Chandru (Lamar Univ., Beaumont, TX), and Jon Pleim (U.S. EPA ORD, Research Triangle Park, NC).

Added a flag to optionally create static output files.

Rationale: As users are focused more on seasonal and annual CMAQ simulations, disk space considerations are more important. Since the information in the GRID files is (for the most part) static, these data do not need to be created with every run of MCIP2.

Impact: Reduces the number of MCIP2 files, if this user option is invoked. Users should be aware that the MM5 non-hydrostatic reference temperature is modified seasonally by some MM5 users, and this will affect the reference height fields (which are used by SMOKE) that are in GRIDCRO3D.

Refined the error-checking for physical discontinuities on MM5 restart runs.

Rationale: MCIP2 unnecessarily stopped users if the MM5 restart and output frequencies were identical.

Impact: Users will not be stopped unnecessarily.

Credits: Luca Delle Monache (Univ. of British Columbia, Vancouver, BC, Canada) identified this problem and suggested the solution.

Added the 10-m wind speed and direction to output.

Rationale: Several MCIP2 users have requested 10-m wind speed and direction for comparison with observations.

Impact: Two fields (WSPD10 and WDIR10) are added to the METCRO2D file. These fields are re-diagnosed in MCIP2 using similarity theory for the 10-m wind speed and assuming no directional shear between the middle of layer 1 and the ground. Some PBL schemes in MM5 make 10-m u- and v-component winds available in the output, and MCIP2 currently ignores those fields.

Added the 2-m temperature to output, if it can be passed through from MM5.

Rationale: To the extent possible, users should have access to variables that are calculated directly in MM5, rather than re-diagnosed in MCIP2.

Impact: One field (TEMP2) is added to METCRO2D output when T2 is available in MM5 output. (The most popular PBL schemes in MM5 now generate T2.) TEMP2 can be used in SMOKE as a replacement for TEMP1P5, but users are cautioned that the re-diagnosed TEMP10 and the MM5-calculated TEMP2 should not be used together in the same SMOKE run.

Added leaf-area index from Pleim-Xiu LSM to output.

Rationale: The field could be handy for downstream processing applications.

Impact: One field (LAI) is added to METCRO2D output when Pleim-Xiu land-surface model is run in MM5.

Credits: Pedro Sanhueza (Univ. of Chile, Santiago, Chile) provided this suggestion.

Enabled MCIP2 to use MM5 output where IFSNOW=2.

Rationale: MCIP2 requires the snow cover field for some of the dry deposition velocity calculations. When MM5 users set IFSNOW=2, the snow cover field is replaced in the MM5 output stream with a liquid-equivalent snow depth array.

Impact: Users can now successfully run MCIP2 when MM5's IFSNOW=2.

Credits: Zion Wang (Univ. of California, Riverside, CA) brought this issue to our attention.

Added explicit calculation of dot-point latitude, longitude, and map-scale factors based on grid geometry.

Rationale: Explicit calculation based on grid geometry is better than horizontal interpolation.

Impact: Some slight differences in dot-point latitude, longitude, and map-scale factors, with more significant differences expected for large domains and domains that are far from the projection's central meridian. (Only map-scale factors are used in the CMAQ system.) Users who change the radius of the earth in MM5 will also need to change it in MCIP2's const_mod.F.

Limited calculation of wind speed for initial time (in MM5 file) to the cross-point domain.

Rationale: The calculation of wind speed for MM5's initial time was based on dot-point winds, even though wind speed is output from MCIP2 on cross points.

Impact: For most users, there will be no impact on MCIP2 runs. This change will result in slight differences in output fields for only the first hour when users start MCIP2 at MM5's initial time (which is generally not done).

Changed local array allocation to occur only on initial calls to subroutines to avoid memory fragmentation.

Rationale: As domain sizes are increasing in the user community, available hardware memory may become more limited. To the extent possible, users should be protected from the potential for memory fragmentation.

Impact: No apparent impact on MCIP2 runs. This modification could prevent segmentation faults with very large domains run for long periods.

Credits: David Wong (Lockheed Martin, Research Triangle Park, NC) identified the potential for memory fragmentation and suggested the fix.

Removed obsolete land-use input options.

Rationale: While the MCIP2 code was apparently set up for six different land-use input options, in practice, the most feasible option is to input dominant land use categories directly from MM5.

Impact: MCIP2 is simplified. In addition, when neither of the re-diagnosed PBL parameter options (LPBL=2 or 3) or the RADM dry deposition (LDDEP=1) is selected, the output dominant land use category (DLUSE) in GRIDCRO2D will be the land use that was used in MM5 rather than the RADM category. DLUSE is not used downstream in the CMAQ system, but users who read DLUSE in a private program should be aware of this change.

Added initialization of I/O API and library checks.

Rationale: For completeness, the I/O API library should be initialized at the beginning of the program.

Impact: Negligible impact on MCIP2 runs.

Credits: David Wong (Lockheed Martin, Research Triangle Park, NC) pointed out the absence of the I/O API initialization.

Updated modules that support I/O API.

Rationale: Since the standard .EXT files in the CMAQ system are F90 modules in MCIP2, they need to be manually updated to be consistent with standard files.

Impact: No impact on MCIP2 runs as these new functions of I/O API are not used by MCIP2.

Added Henry's Law constants for new species.

Rationale: The Henry's Law constant routine in MCIP2 was adapted from the same routine in CMAQ. These routines should be kept consistent.

Impact: No impact on MCIP2 runs.

Credits: Donna Schwede (U.S. EPA ORD, Research Triangle Park, NC) identified that the two hlconst.F routines had diverged.

Removed bookkeeping XFLAGS arrays.

Rationale: The XFLAGS arrays were designed to keep track of which routines filled the output arrays. They are not used, in practice.

Impact: No impact on MCIP2 runs. Simplifies code and future modifications to the code.

Eliminated type mismatches flagged by compiler.

Rationale: Good coding practice suggests that there should be no "type mismatches".

Impact: No impact on MCIP2 runs as the affected routine (ratint.F) is currently unused.

Eliminated support for NT version of MCIP2.

Rationale: As far as we know, no one is using it.

Impact: No impact on MCIP2 runs.

3. ANTICIPATED FUTURE MODIFICATIONS

A major upgrade to MCIP will enable the capability to use output from the Weather Research and Forecast (WRF) model. A preliminary version has been developed at the Institude for Multidimensional Air Quality Studies at the University of Houston, and that version will most likely form the template for the upgrade to MCIP. A minor improvement to MCIP will include an option to process dry deposition velocities for toxic

species to support a CMAQ release that models toxics. Also, now that it is common for researchers to modify their I/O API libraries to accommodate more than the "default" 120 species maximum (e.g., for aerosol or toxics research), a check will be inserted to ensure the I/O API libraries are dimensioned consistently with the MCIP2 code will prevent the code from crashing for this reason. The latter change will be implemented following an official release of I/O API Version 3 by Baron Advanced Meteorological Systems.

If users have made changes to MCIP that they believe would benefit others in the user community, they are encouraged to submit those changes to CMAS for consideration for an upcoming release of MCIP.

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