Participant Call February 8, 2024

Participants: Richard Kranenburg, Christian Hogrefe, Ummugulsum Alyuz, Paul Makar, Jesse Bash, Kenjiro Toyota, Annika Vogel, Roberto San Jose, Olivia Clifton

Grid intercomparison (Activity 1)

- Model data updates:
    - 10700 and 10701: While reviewing Paul's manuscript, Christian discovered a serious error in his post-processing of CMAQ M3Dry and STAGE NH3 net dry deposition fluxes. During the variable renaming and unit conversion from kg/ha to eq/ha , these fields were not divided by the molecular weight and the reported fields were therefore too high by a factor of 17. The erroneous expression used was "DFLUX-NH3 , eq ha-1, 1000.*(DDEP_NH3_Flux[1]/)*1." while the correct expression should have been "DFLUX-NH3 , eq ha-1, 1000.*(DDEP_NH3_Flux[1]/17.)*1.", and unfortunately the omission of the molecular weight in the denominator did not trigger a warning or error in the code parsing and applying these expressions. This omission of the molecular weight was isolated to the post-processing of this particular species. As a result of these erroneous fields, Paul's analysis identified NH3 dry deposition fluxes as leading cause of ensemble variability in N deposition over NA, and also as leading contributor to N deposition for CMAQ. Christian created corrected fields and uploaded them, these new fields bring CMAQ results in line with other models and no longer identify NH3 dry deposition as the leading cause of ensemble variability. Paul has recalculated the total N deposition fields for the two CMAQ runs and the reduced ensemble and shared them with the groups performing the critical load exceedance calculations which need to be updated in the manuscript.
    - 10707: Richard has updated the LU information (missed some ag land) on the sftp server and is re-running the diagnostics with the corrected LU information.
    - 10708: Roberto has recalculated effective conductances and fluxes using an approach proposed by Paul to overcome inconsistencies between the code in WRF/Chem and the post-processing code relating to limit values. The recalculation has been completed for all cases for all pollutants except SO2 and NH3 for the grid scale values, including a fix to the units for O3, HCHO, and H2O2 identified last month. The calculation for LU-specific values has been completed for the two NA cases and will be completed within the next day or two for the two EU cases. The recalculations for SO2 and NH3 will be performed in the near future after Roberto and Paul identified a viable approach for those pollutants.
    - 10709: Several email exchanges occurred regarding the following issues:
        - "Stripiness" in many deposition-related output fields: these have been identified as having been caused by discontinuities in the fields that were used to assign a given grid cell in a given simulation month to the five "seasons" used in the WRF/Chem Wesely scheme. Therefore, the origin of this behavior was prior to the WRF/Chem runs being performed and cannot be resolved by applying post-processing fixes. Essentially, in some months, some adjacent grid cells were being assigned to unrealistic Wesely scheme "seasons", yielding discontinuities in dry deposition diagnostics, but also affecting the actual WRF/Chem simulations
        - Resolution of LU fraction questions:
            - 10709 used MODIS in the NOAH LSM, but for the Wesely deposition code calculations in WRF/Chem, these were mapped to USGS24 (which were then

reported to AQMEII4 as NATIVELANDUSE##) and those were then mapped to the 16 AQMEII4 categories (REPTRDLANDUSE##) when reporting LU-specific diagnostics and aggregating them to the grid cell. This means that while all WRF/Chem models (10702, 10708, and 10709) worked with the 24 USGS categories in the dry deposition code, they differ in the underlying LU input to the model (USGS24 for 10708 NA and EU, USGS24 for 10702 NA and USGS24+CORINE for 10702 EU, MODIS for 10709) and LSM.
        - The presence of multiple LU categories with fractional coverage > 0 for 10709 noted in last month's call was not the result of a fractional LU coverage / mosaic approach in the LSM, but rather an artifact of the regridding of the reported fields to the common AQMEII4 grid. In contrast to other models that used conservative regridding for concentrations, fluxes and meteorology and nearest neighbor regridding for all dry deposition diagnostic fields, all 10709 regridded fields were generated with conservative regridding. This means that all WRF/Chem models used a dominant LU category modeling approach.
    - Internal inconsistency between O3 Vd and sum of ECOND: This issue is still unresolved
- Data storage updates:
    - No updates since the last call
- Analysis updates:
    - Paul has received co-author comments on the draft manuscript. Extensive revisions are needed due to the CMAQ NH3 dry deposition error noted above
    - Christian continued the analysis of the ozone dry deposition diagnostics (grid-scale and LU-specific) and LU information submitted by all groups and showed a draft manuscript outline and collection of potential figures

Point intercomparison (Activity 2)

- An Activity 2 call was held on February 6. Anam and Annika presented updates on their ongoing work.
- Olivia, Stefano, and Christian had a call with the HTAP organizers on January 12 to discuss how experiences from AQMEII4 (and TOAR) can inform the upcoming HTAP OPNS simulations. For its planned modeling and impacts (ozone damage to plants) work, HTAP3 may use a different approach to estimating stomatal ozone dose (top of canopy, sunlit only) from what is being calculated in typical CTM deposition schemes, likely because this approach is easier to link to chamber studies. Such calculations require multi-layer models rather than information that most current deposition schemes can provide, though it might be possible to find relationships between that approach and the approach in most deposition schemes.

Check-in on AQMEII4 special issue (submission deadline July 31, 2024)

No updates since the last call to the list of published and planned manuscript below

- Galmarini et al. (2021) Activity 1 overview technical note - published (https://acp.copernicus.org/articles/21/15663/2021/)

- Hogrefe et al. (2023) analysis of EPA CMAQ NA simulations - published (https://acp.copernicus.org/articles/23/8119/2023/)
- Clifton et al. (2023) Activity 2 overview manuscript - published (https://acp.copernicus.org/articles/23/9911/2023/)
- Additional planned and potential manuscripts:
    - Activity 1: Makar et al. – critical loads ensemble analysis - draft circulated to co-authors
    - Activity 1: Toyota et al. updates to GEM-MACH - how can results from Activity 2 be used to check/update the representation of dry deposition in regional modeling. Final decision on whether or not a manuscript will be developed to be made by spring 2024.
    - Activity 1: Kioutsioukis et al. – multi-model operational evaluation and analysis of AQMEII4 grid models – Stefano and Iannis iterating on figures
    - Activity 1: Hogrefe, Galmarini, Makar, Kioutsioukis et al. - multi-model analysis of ozone dry deposition diagnostics (grid-scale and LU-specific) and LU information – work is ongoing, target for draft manuscript: spring 2024
    - Activity 1: Lee, Soares, Makar, et al. – use of hierarchical cluster analysis for grid model intercomparison
    - Activity 2: Khan, Clifton, et al. – observational constraints on stomatal conductance and point model sensitivity simulations
    - Activity 2: Lee, Makar, et al. – use of meteorological cluster analysis for point model evaluation
    - Activity 2: Lee, Makar et al. – physics-informed machine learning for potentially refining point model parameter values
    - Activity 2: Vogel et al. - statistical error estimation analysis
    - Activity 2: Bash et al. – use of AQMEII4 flux measurement for optimization of selected STAGE resistances. Writing planned for spring 2024.

Next call March 14, 2024