

Participant Call September 14, 2023

Participants: Rohit Mathur, Ummugulsum Alyuz, Christian Hogrefe, Jesse Bash, Kenjiro Toyota, Paul Makar, Olivia Clifton, Stefano Galmarini, Colleen Baublitz

Grid intercomparison (Activity 1)

- Model data updates:
 - 10707: August call recap: Christian noted that he had downloaded, processed, and visualized the EU2009 LU-specific dry deposition diagnostic files and still saw some inconsistencies between the sum of the effective conductances and the deposition velocity. Richard said he would look into it. Richard also noted that he had uploaded EU2010 which Christian then downloaded after the call. No further updates were received since then.
 - 10712: No updates since the last call, no data received yet.
- Data storage updates:
 - No updates since the last call
- Data extraction and analysis updates:
 - After the last call, Paul, Philip, and Christian discovered an issue with 2016 SO₂ observations over Canada which had been used for the receptor extractions:
 - the Canadian hourly SO₂ observations for 2016 somehow were too low by a factor of 10 – we suspect a unit conversion issue somewhere along the way, where the original data was actually in tens of ppb but being interpreted as ppb. The Canadian data for this case are those for stations starting with NAPS while the US data (unchanged) are those for stations starting with AIRS.
 - Paul generated a new, corrected set of NAPS hourly SO₂ data for 2016. Christian then created a new tar file with these observations (along with the exiting .info and .tm files) and uploaded it to the sftp site.
 - Christian also created new tar files with model extractions for all eight simulations – not because the actual extractions changed, but only because Paul's new corrected NAPS hourly SO₂ data set for 2016 contains two fewer sites than the original data set. So, for consistency, those two same sites (NAPSCANONBRN and NAPSCAON1CNT) were removed from all model extractions as well.
 - Summary of changed tar files:
 - SO₂_OBS_0251_001_hourly.tar.gz
 - Updated values for NAPS* stations in all files (correcting the factor of 10 error), no changes to AIRS* stations
 - Removal of data for NAPSCANONBRN and NAPSCAON1CNT
 - SO₂_{model}_0251_001_01_01.tar.gz
 - Removal of data for NAPSCANONBRN and NAPSCAON1CNT
 - Paul is currently double checking if other pollutants may be affected, too, though an initial quick glance suggests that this may be limited to hourly SO₂ from NAPS.
 - Paul is also exploring whether NAPS observational data for 2010 could still be prepared (currently 2010 hourly gas phase and aerosol data is for the US only). If so, Christian

would create updated pool files and start extracting model output for this larger set of sites, resulting in new files for 0241/001/*/01.

- In July, Paul, Stefano, and Christian started having separate monthly calls review progress on analyzing the ozone dry deposition diagnostics (grid-scale and LU-specific) and LU information submitted by all groups and scope out a manuscript based on this analysis. Christian has started this analysis, initially focusing on reviewing the land use information reported by all groups. Christian showed a few slides illustrating the land use analysis performed to date.
- Paul showed slides to provide an update on the sulfur and nitrogen deposition and critical loads paper he is writing. There were also some two follow-ups on the August SO₂ model evaluation discussion that noted that the models have high bias over NA but generally not over EU (at least at EMEP sites):
 - See discussion above regarding updates to SO₂ observations over Canada
 - Role of point source plume rise and emission vertical allocation:
 - Richard noted that TNO had provided reference vertical allocation profiles (used in LOTOS-EUROS) to all groups via the AQMEII4 github site at <https://github.com/AQMEII4/Activity-1-AQMEII-style-runs/blob/master/EU%20emissions%20temporal%20profiles.zip>
 - Christian sent an email to WRF/Chem groups asking for details on their approach to point source vertical allocation, both over NA (where stack information was available) and EU (where point source / power sector emissions are provided as 2D files and groups need to implement an approach to vertical allocation)
 - Roberto: EU simulations: We have used a vertical profile per emission category (table), specifically the recommended table for TNO/CAMS emission inventory is based on: J. Bieser, A. Aulinger, V. Matthias, M. Quante, H.A.C. Denier van der Gon, Vertical emission profiles for Europe based on plume rise calculations, Environmental Pollution, Volume 159, Issue 10, 2011, Pages 2935-2946, doi:10.1016/j.envpol.2011.04.030. NA simulations: 2016: NCL script "AQMEII project emissions converter; Christoph Knote, NCAR, ACD, 03/28/2013". 2010: NCL script "AQMEII project emissions converter; Christoph Knote, NCAR, ACD, 03/28/2013" + Corrections of plume rise calculations (corrected as directed by Hogrefe mail Wed, 20 Apr 2022 14:58:17 +0000 based on mail from Barron H. Henderson). + Corrections of fire emissions (Post of Young-Hee Ryu Wed, 20 Apr 2022 00:46:17 +0900 based on Hodzic et al. (2007) and using the variable ACRESBURNED).
 - Aura: For EU simulations, I applied the vertical emissions profiled from the plume rise model of Bieser et al., 2011. It is a standard profile used at the European level and it was provided by TNO (<https://essd.copernicus.org/articles/14/491/2022/>). There is no change between the vertical profile used by the TNO-MACC-III emissions inventory and the one used by the CAMS-REG-ANT inventory.

- Previous (2022) email documentation on WRF/Chem plume rise issues, affecting all WRF/Chem NA runs except 10708 NA 2010 (performed after issue was discovered):
 - All WRF/Chem groups used a script developed by Christoph Knote for AQMEII2 to estimate plume rise from the CMAQ-ready point source files distributed to modeling groups, utilizing stack variables from those files
 - In spring 2022, several issues were discovered: 1) the plume rise equations did not properly implement the Carson and Moses (1969) approach referenced in the script, 2) plume rise for fires was treated the same as plume rise for anthropogenic sources rather than making use of the burn area information available in the files, and 3) the stack flow information in the input files and used by the script was incorrect, using the stack flow of the last source in the file for all sources.
 - The errors for issue #1 happen to mostly cancel out each other. Issue #2 affects 10708 for NA2016 and 10702 (Aura) for NA2010 and NA2016, but not 10709 (Alma/Younghee) because they updated the script to treat wildfire plume rise differently. Issue #3 affects all previous WRF/Chem simulations, the effect is random. For his current NA2010 WRF/Chem runs, Roberto is using stack exit velocity and diameter to recompute flow.
 - The CMAQ and GEM-MACH runs were not affected by any of these issues. CMAQ uses stack exit velocity and diameter to compute stack flow rather than using the (erroneous) stack flow information from the files. Paul's group performed their own SMOKE processing (using the same SMOKE inputs as those used to create the CMAQ-ready files distributed to all groups) rather than using the CMAQ-ready files.
- Colleen shared that she is planning diagnostic analysis of wet deposition fluxes, potentially including additional model (CMAQ, maybe GEM-MACH) sensitivity simulation exploring the representation of multiphase scavenging. Her work would build off of results presented in Paul's paper and include analysis at regional and sub-seasonal scales.
- Colleen also provided an update from the NADP community about Bret Schichtel's group at the National Park Service planning to perform 2016 CMAQ and CAMx simulations with common inputs to compare simulated estimates of nitrogen deposition. While the inputs of these simulations differ from AQMEII4 and model outputs to not include the AQMEII4 dry deposition diagnostics, there may be interest in comparing results for fluxes and concentrations in the future. Christian noted that there had been efforts to include Bret's group in AQMEII4 but this ultimately did not work out due to timing and resource considerations.

Point intercomparison (Activity 2)

- An Activity 2 call was held September 5. Olivia's paper has been published. Anam Khan presented a list of proposed sensitivity simulations to further analyze effective stomatal conductances, stomatal conductance to ozone, and stomatal uptake of ozone simulated by the point models and comparing them to the observational datasets participating in AQMEII4. The

sensitivity simulations involve setting different values for parameters and stress functions related to water stress. Anam sent out a detailed list of the proposed simulations to all point modelers on September 12, asked for feedback by Monday September 18 on whether modelers would be interested in participating, and proposed a deadline of October 6 for submitting the results of the sensitivity simulations.

- Olivia also participated in a recent TOAR2-deposition call and provided an update on the AQMEII4 point intercomparison work, including plans for Anam's future work. TOAR2 focuses on point model simulations at Fluxnet ag, forests and grassland sites (use measured carbon and water vapor fluxes, not ozone fluxes). Their analysis will look at seasonal ozone flux profiles and sensitivity towards meteorology, and maybe LAI and growing season timing. TOAR2 call participants asked if Anam's work could guide their analysis, Olivia will discuss this further with Anam to make sure the timing is right and her input would be credited appropriately. Oliver Wild may conduct some Monte Carlo analysis for parameter testing, this might partially overlap with Jesse's work (though that is for STAGE which does not participate in TOAR2) and the AQMEII4 work by Kenjiro and Colin - Leiming will coordinate with his ECCC colleagues to avoid overlap.

Special issue - submission deadline extended to July 31, 2024

- 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 / potential manuscripts:
 - Activity 1: Makar et al. – critical loads ensemble analysis – Paul continues to work on the draft
 - Activity 1: Makar et al. potential updates to GEM-MACH - how can results from Activity 2 be used to check/update the representation of dry deposition in regional modeling. Paul will lead this, but not until after finishing the critical loads analysis, i.e. not before September.
 - Activity 1: Kioutsioukis, Galmarini et al. – multi-model operational evaluation and analysis of AQMEII4 grid models – Stefano reported that there has been no recent progress, but he plans to start working on it full time soon
 - Activity 1: Hogrefe, Galmarini, Makar, Kioutsioukis et al. - multi-model analysis of ozone dry deposition diagnostics (grid-scale and LU-specific) and LU information - Christian will start this analysis and Paul, Stefano and Christian will have monthly calls to review progress and scope out a draft manuscript. Target: winter 2023/2024
 - 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: Bash et al. – use of AQMEII4 flux measurement for optimization of selected STAGE resistances. Jesse aims for draft in late fall, early winter

Next call October 12, 9:00 EDST / 13:00 GMT / 14:00 BST / 15:00 CEST