Activity 2 Participant Call May 7, 2024

Participants: Jesse Bash, Olivia Clifton, Stefano Galmarini, Christian Hogrefe, Annika Vogel, Johannes Flemming, Laurens Ganzeveld

Olivia reported that she expects Anam to provide an update on her draft manuscript after her PhD defense this month.

Jesse presented results from his work to use the point intercomparison observational data to optimize the representation of non-stomatal (cuticular and soil) conductance in STAGE. The optimization is using the Nelder-Mead method to minimize the Symmetric Median Absolute Percentage Error (SMAPE) in both deposition velocity and deposition flux (concentration-weighted deposition velocity). The observational dataset is divided into 11 subsets for a 10 fold cross validation. At its current stage, the stomatal conductance is not included as a target in the optimization approach. The framework for the revised representation of cuticular and soil resistances in STAGE was adapted from GEOSChem. The representation of cuticular conductance includes a dependence on leaf mass per area which can serve as an indicator of plant functional type (e.g. herbaceous vs. evergreen) because of its correlation with the carbon to nitrogen ratio of the vegetation. The soil resistance in the framework is assumed to be a constant. Using the optimization technique to identify parameter values for the cuticular and soil conductances in that framework that minimize SMAPE identifies an entire range of points that falls along a curve with an inverse relationship between Rsoil and Rcut. The point corresponding to the Rsoil and Rcut values used in the current STAGE version implemented in CMAQ does not fall onto that curve, indicating room for improvement. Since there is not sufficient information in the observational data to identify a single best combination for Rsoil and Rcut, Jesse then selected three values for the constant value of Rsoil (low, medium, and high) and the corresponding Rcut values from the curve of minimum SMAPE, and then used these 3 different versions of revised STAGE in hemispheric CMAQ simulations. Comparing ozone concentrations from these three simulations with revised STAGE against observed concentrations from TOAR2 and AQS shows a clear improvement in correlations and error relative to a simulation using the base STAGE model. Improvements were especially noticeable in areas with lower vegetation coverage, indicating that the soil uptake in the current implementation of STAGE is too high.

In the discussion of Jesse's results, Laurens noted that these optimizations of the non-stomatal components might still depend on the representation of stomatal uptake, and that splitting the cuticular vs. soil terms involves inferring the location of the canopy sink versus the soil sink which is sensitive to the characterization of the in-canopy turbulent transport terms. He also wondered whether the revised framework (which assumes a constant value for Rsoil and represents Rcut as a function of leaf mass per area) is suited to take into account effects of

variations in soil moisture and organic material on Rsoil and variations in canopy wetness on Rcut.

Regarding the discussion of stomatal uptake effects on Jesse's work, he and Olivia will follow up to explore whether incorporating the observational constraints on stomatal conductance prepared by Anam into his work might help to further refine revisions to STAGE. Sharing these stomatal conductance estimates is not expected to happen before Anam's defense.
The group then had a brief discussion on a slide shared by Jesse in which the ozone concentrations from his hemispheric CMAQ simulation showed a significant underprediction of observed concentrations during springtime. Such underprediction is also seen in some other global models, and the question was raised whether errors in ozone dry deposition might be a factor. The groups initial sense was that these errors are more likely related to the representation of dynamics, stratosphere/troposphere exchange, and chemistry (e.g. aerosol nitrate photolysis), but no definitive conclusion was possible.

Annika reported that she will present her ongoing work on statistical error estimation at a workshop on sensitivity analysis and data assimilation at the end of May. She then shared draft slides that illustrate the application of her mathematical approach to the AQMEII4 point intercomparison dataset. The presentation focuses on the importance of carefully selecting the assumptions about error correlations that are required by her approach. While the assumption that observational errors are uncorrelated to errors in the point models likely is justified, the approach requires one further assumption of one pair of point models also having uncorrelated errors. The slides she presented illustrate that arbitrarily selecting the pair of point models for which this condition is assumed to be true can yield unrealistic and un-interpretable results. In her most recent work, she developed a formal methodology for selecting the pair of point models assumed to satisfy this conditions. Applying this new methodology to the data set at one example site yields results that allow for a meaningful analysis of error relationships between the different point models as well as observations.

Finally, the group briefly discussed the timeline for the special issue and supported the proposal made during the April 18 Activity 1 call to ask Copernicus for a one year extension of the deadline. A final decision about when to request that extension was expected during the May 9 Activity 1 call. In the future, Activity 2 calls may move to occuring bi-monthly or possibly on an as-needed basis, this will be discussed further during the next call.

Next call: June 4.