Participant Call October 12, 2023

Participants: Jesse Bash, Annika Vogel, Christian Hogrefe, Paul Makar, Colleen Baublitz, Kenjiro Toyota, Olivia Clifton, Rohit Mathur, Ummugulsum Alyuz, Jon Pleim

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 August call.
        - Email follow-up 10/12/2023: Richard is looking into this, it may come down to their reported ECOND-SOIL including their reported ECOND-LCAN and not weighting either term by the vegetation fraction, like M3Dry and STAGE do. Christian to follow up with Richard, Paul, and Olivia after the call

- Data storage updates:
    - No updates since the last call

- Data extraction and analysis updates: While working on the sulfur and nitrogen deposition paper, Paul came across issues with a few diagnostic fields from some WRF/Chem simulations, these were communicated back to Roberto, Aura, Alma, and Young-Hee:
    - 10702: potential units and lower limit cut-off issues for EU 2010 effective flux data for HNO3 (0351-042-15,16,17,18).
        - As of October 12, no response has been received yet.
    - 10709: error in model post-processing or model output, array overflows in the output field. I'm hoping that this is something that happened in 10709's post-processing of the model output as opposed to the model output itself. The issue is easiest to see with a logarithmic color scale for 10709's TSD -0251-002-042-15, and TSD-0251-002-042-18, but might be in -042-15 and -042-16 as well. When you plot the gridded model values with a logarithmic color scale, parallel lines of higher values show up along lines of latitude. This sort of thing usually occurs when an array size error is taking place; I'm hoping its not in the original model output and is in the post-processing and hence correctable. [Added by Christian]: this appears to be not just be in the effective flux variables 15 – 18, but also the corresponding effective conductance variables 06 – 09, e.g. 10709-0251-042-06
        - Young-Hee responded via email before the call and said she would investigate this issue and would get back to Paul.
    - 10708:
        - Issue #1: For the 012 – 122 TSDs that contain the grid-scale diagnostics, the -09 effective conductance fields and -18 effective flux fields for the soil pathway are consistently not present for 012 and 052, i.e. SO2 and NH3, while they are consistently present for all other pollutants (except that nothing is being

reported for 092 ONIT). We also checked the LU-specific TSDs 132 – 442, and the effective conductances for these species (we don't have LU-specific effective fluxes) are not reported as well, so this is all internally consistent

- Issue #2: TSD 0251-042-17, TSD 0351-042-17. Magnitude error for the effective flux for HNO3 for the cuticle resistance pathway. Two of the other pathways {lower canopy (042-15), stomatal (042-16) } seem to be ok; the range of values is from zero to about 600 eq ha-1 yr-1, which is equivalent to the other models. However, for 042-17, the range of reported values is roughly from 1x106 to 1x109: 042-17 is about 1x106 higher than the other pathways.
- Issue #3: The values of TSD-0251-042-18 (soil pathway) also seem to incorporate some very high values. A possible reason for these large numbers might be division by a low-number cut-off to prevent division by zero being used somewhere in the creation of the effective conductances or fluxes, perhaps inconsistently, in the effective conductance formulae. The other effective flux numbers for this model (-15, -16) all seem reasonable and similar to those of the other models. It could be the same issue affecting this model's values for 0251-042-17 and 0251-042-18, with the -17 being affected by that cutoff value more frequently.
- Email follow up by Roberto: We already discussed this in a mail of 03/15/22, where Christian asked us about " "10702 and sometimes 10708 have very large values for some pathways for HNO3, HNO4, and N2O5". On that occasion we replied: "About the conductance peaks for HNO3, HNO4 and N2O5, sometimes, we have observed that the cuticular resistance rcut has very low values (e-5 approx.) for those pollutants (in particular when we have rain or humidity > 95%). Just these pollutants have very high values for Henry constant (e+13). These cuticular resistance values should make that the surface resistance RC values to be very low (e-5), but in the WRF/Chem model code, the Rc is limited to 100 (s/cm) so that the cuticular resistance (ECUT = (1/rcut)*Rc), instead of using a value in the order of c-5, the model is using a value of 100, so that we obtain large values of the cuticular resistance." The explanation is not exactly what Paul is talking about but it does go in the right direction. In addition the effect is more visible in areas of high humidity, ("coastlines and over parts of the western mountain ranges in the USA."). As in the simulation, what is saved is the Rc already limited to 100, we could not obtain the original Rc in the cases < 100 to recalculate the Ecut. For now we can't think how to solve it without re-running model, we will think about it with some more time in case we can think of something, suggestions are welcome.
- Email follow by Paul: thanks for the reminder that it's come up before. So, if I understand this correctly (please confirm):
    - Internally, in the gas-phase dry deposition calculations, very low surface resistance values are sometimes calculated, due to very low cuticular resistances.
    - Subsequent to that calculation, the calculated value of Rc is subject to a Rc = max(Rc, 100 s/cm) value.
    - What was output in the diagnostics for Rc was the value after step (2). Same for Vd; it's the post-cutoff value.
    - However, the value of rcut is the original value of rcut from within the deposition code, and no cutoff was applied there.

- So the problem is occurring due to a post-cutoff value of Rc being combined with a pre-cutoff value of rcut… with the result being the very large values in the ECOND and DFLX diagnostics wherever the cutoff happened to be applied.

So the question in this case is "How do we ascribe the relative mass fraction to the different pathways when the final result, the Rc and Vd values, have been subject to a minimum Rc value cutoff?"
I think that this could be done relatively easily from the existing model output, without having to do a rerun (thank goodness!!). 😊 The basic underlying idea is "Assume that, when a lower limit cutoff has been applied to Rc, that the relative pathway fractions are the same as the non-cutoff value of Rc".
So, in the case of model 10708, and with reference to table B6 in Galmirini et al, you would

- Divide the hourly ECUT, ESTOM, ESOIL and ELCAN values by the corresponding values of (Rc * Vd), where the Rc and Vd values are those reported and derived from the use of the cutoff. Carrying out this action for each effective conductance, this would return the pre-cutoff values of$1/r_cut$, $1/(r\_m+r\_s)$,$1/(r\_ac+r\_gs)$, and$1/(r_dc+r_cl)$, respectively.
- You then calculate a new pre-cutoff value of Rc, let's call it Rc*, from the above values from step (1):
  $R\_c^*= 1/(1/r\_cut +1/(r\_m+r\_s)+1/(r\_ac+r\_gs)+1/(r\_dc+r\_cl))$
  Note that this value ofR_c^* (and its components) are not subject to the cutoff, yet for places where theR_c^* value does not happen to fall below the cutoff, Rc* = Rc.
- You then recalculate the effective conductances, but this time use Rc* in the numerator, for example, for the cuticle effective conductance:
  $E\_CUT=(R\_c^*)/r\_cut \ V\_d$
  Note that the Vd value in the above equation is the reported post-cutoff value: we are making the assumption that in the event of a cutoff, the relative contributions to the net deposition velocity would be the same. Where the cutoff has not been applied, the resulting value of ECUT would be exactly the same as before. Where the cutoff has been applied, the big values will be gone, making use of the inference that the relative importance of the pathways is the same, for post-cutoff and pre-cutoff Vd.
- You then use the revised ratios like$(R_c^*)/r_cut$ to recalculate the effective fluxes (DRYFLUX variables, Table 4 of Galmarini et al). Same deal as for (3): you'll get the same values as before for locations above the cutoff, and the large values for below cutoff will be gone.
  So – this can be done as post-processing of the existing output, I think. The issue that we didn't recognize in the protocol was

"what happens when the net resistance has an imposed lower limit?". I think a reasonable and defendable answer is "We assume that the relative fractions of the different pathways would still apply" – and modify the calculation accordingly. This would remove the ambiguity associated with the very high values – and can be done entirely with a little bit more post-processing of the existing hourly values used for the submitted variables. What do you think? Can please you give this a try? It would give more consistent results and allow users of the database to correctly infer the relative importance of the pathways to the deposition velocities and fluxes within the cutoff regions.

- Email follow by Roberto:
  - We have uploaded the data files of the ECOND-CUT (08) and DFLX-CUT(17) variables for the pollutants NO2(22), NO(32), HNO3(42) and PAN (62) to the AQM SFTP server (folder 10708), after correction of the cut-off effect of the Rc (in the model it is limited to 100), using the "algorithm" proposed by Paul Makar (based on re-calculating the Rc without cut-off and using this new Rc to calculate ECOND-CUT and then DFLX-CUT). … The values now look consistent and those 10^8 peaks no longer appear.
  - For the pollutants NH3 and SO2 we cannot apply the algorithm because there was a problem (NaNs) in obtaining the ECOND-SOIL values in the model run.
  - The files for the NA-2016 case have been uploaded (it is the one we had more easily accessible). Please take the new data and see if it is consistent with other models. If we receive the OK, we would move on to produce with the same scripts, the remaining pollutants and the remaining case studies (1 more NA and the 2 EU). Meanwhile we will be loading the original data in our computer from the backup disks where we have the information to be able to run the scripts.

- During the call, Christian asked Paul to please go through these emails, check if Roberto's latest response addresses all the three issues initially raised by Paul, and then follow up with Roberto.

- 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 is continuing this analysis, initially focusing on reviewing the land use information reported by all groups.
  - Some updates for a few GEM-MACH fields are expected based on initial results of this analysis:
    - 10703: z0 needs to be regenerated.
    - 10704: z0 and the land-use fields need to be regenerated
    - 10705: z0 needs to be regenerated.

- Annika Vogel of Environment and Climate Change Canada introduced herself to the group and proposed to apply a method she recently developed to AQMEII4 data sets. She prepared and shared several slides describing the method listing potential follow-up analyses.
    - The method is based on a new approach to estimate error statistics of multiple data, so the multi-model output and measurement data in the AQMEII4 project would be a very interesting application. The method can be applied to any set of datasets which contain information about the same quantities. It is especially tailored for a large number of datasets which cannot all to be assumed to have uncorrelated errors. In turn, the more datasets are used, the more error cross-covariances (ie correlated errors between datasets) can be estimated. Its application to multi-model ensembles and validation observations would be very interesting: Despite estimating statistical covariances (incl spatial and cross-species correlations, depending on the availability of observations) of all datasets, it could provide an idea on how much the errors of different models are correlated (in a statistical sense).
    - Olivia noted that applying this method to the Activity 2 datasets could indeed be very interesting, complementing the application of other statistical tools to CMAQ-STAGE (Jesse) and GEM-MACH (Colin and Kenjiro) dry deposition schemes.
    - Christian also thought that the application of this method to the Activity 1 datasets would be of interested, taking into account work on similar topics performed by Stefano, Iannis, and their colleague Efisio Solazzo during previous phases of AQMEII.

Point intercomparison (Activity 2)

- An Activity 2 call held on October 2, call notes have been posted to the github site.
- Olivia reported that she recently attended the CCMI meeting in France. While she did not present on AQMEII4, she was approached by several people who told her that they considered the process-oriented approach to analyze dry deposition employed in AQMEII4 to be very useful
- Olivia also followed up with the co-chairs of HTAP (Tim Butler and Terry Keating) about how the type of dry deposition diagnostics employed during AQMEII4 could be part of the planned HTAP modeling experiments. While those simulations are focused on CH4 impacts on ozone and source apportionment approaches, there is interested in incorporating process-oriented deposition diagnostics. Olivia will continue to coordinate with Tim and Terry.
- Olivia reported that Anam is collecting contributions from sensitivity runs and that some modelers need some more time. She already has some results and started analyzing them. She will prepare an AGU talk based on these results and will have parts of it ready for discussion at the next Activity 2 call.
- Olivia also reported that she continues to work with Nicole Ruiz on the Bugacpuszta analysis.
- Kenjiro reported that he developed an update to the GEM-MACH Wesely deposition scheme that incorporates a dependence on soil moisture dependence for stomatal conductance. Paul is testing this in a high-resolution model application.
- Jesse reported that he finished all STAGE calibration runs for his manuscript updating selected STAGE parameters and plans to start writing after AGU.

NADP TDEP Committee Meeting: Paul noted that he was invited to give a talk on his work at the October 24 NADP TDEP committee meeting.

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
    - 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. – physics-informed machine learning for potentially refining point model parameter values
    - Activity 2: Lee, Makar, et al. – use of meteorological cluster analysis for point model evaluation
    - Activity 2: Bash et al. – use of AQMEII4 flux measurement for optimization of selected STAGE resistances. Finished all calibration runs, will start writing after AGU.

Next call November 9, 9:00 EST / 14:00 GMT / 15:00 CET