

AQMEII4 Activity 2 Call Notes, 11/07/2023

Participants: Olivia Clifton, Stefano Galmarini, Kenjiro Toyota, Annika Vogel, Laurens Ganzeveld, Jesse Bash, Colin Lee, Roberto San Jose, Anam Khan, Chris Holmes, Christian Hogrefe

Colin Lee presented his ongoing work on using physics-informed machine learning to study the relationships between the measured meteorological parameters and measured deposition velocities at the eight ozone flux measurement sites. The slides were an expanded version of his presentation at the CMAS conference in October. Colin first showed that when using the GEM-MACH Wesely scheme in its current form, the correlation between predicted and observed ozone deposition velocities across all sites and hours was 0.37. When applying a “black box” neural network without any physical constraints, the correlation improved to 0.83 and the RMSE was reduced by a factor of 5 compared to using the GEM-MACH Wesely scheme. Colin then constructed a combined set of three neural networks that follow the Wesely approach of representing deposition velocity as the inverse of the sum of three component resistances (r_a , r_b , and r_c), and further constraining the three individual sub-networks for r_a , r_b , and r_c to only use the set of meteorological input variables used in the calculation of these resistances in the GEM-MACH Wesely scheme. This physics-informed neural network had a correlation coefficient of 0.78 and a RMSE comparable to the “black box” neural network, indicating that there is potential for this approach to further explore and potentially update relationships between input parameters and deposition velocities in a physically meaningful manner. In future work, Colin plans to explore further breaking down the r_c term into its stomatal, cuticular, lower canopy, and soil components. To potentially expand this analysis to land use types beyond those covered by the eight flux measurements sites, call participants also suggested that other, shorter-term datasets may be available. In addition, potentially expanding the analysis to pollutants besides ozone (HNO_3 , SO_2 , H_2O_2) might help better constrain some of the component resistances. For example, Jesse noted that potentially working with HNO_3 datasets might help better constrain relationships between input variables and r_a and r_b since those are the dominant resistance terms for that pollutant. Olivia noted that Eiko Nemitz’s group is performing multispecies flux measurements.

Anam showed initial results from her analysis of the first set of point model sensitivity simulations that had been submitted (STAGE, GEM-MACH, and TEMIR). She noted that more recently she had also received result from UPM and ECMWF and was still processing them. Commenting on Anam’s initial results, Laurens suggested that it might be interesting to stratify the analysis between models that use the same approach to account for vapor pressure deficit effects on stomatal conductance (which might point to implementation uncertainties) versus models that use different approaches to account for moisture stress impacts on stomatal conductance. Anam will present her analysis at the AGU meeting in December and plans to go over her slides with the group during the next Activity 2 call on December 5.

Next call: Tuesday December 5, 10:00 EST / 15:00 GMT / 16:00 CET