Activity 2 Participant Call March 7, 2023

Participants: Olivia Clifton, Laurens Ganzeveld, Paul Makar, Stefano Galmarini, Colin Lee, Christian Hogrefe, Jesse Bash, Jon Pleim, Johannes Flemming

Activity 2 Overview Manuscript: Olivia reported that she has been working on strengthening the conclusions and takeaway messages. She also noted that all groups she had contacted with various documentation questions have provided the requested information. One group is rerunning their model and is expected to provide updated results imminently. To reduce page charges, the material contained in the appendix will be published as supplemental material instead. After receiving management approval, Christian has initiated the process of having his division cover the page charges which are expected to be billed sometime later this year, after the manuscript is accepted for final publication. Paul noted that his division might also be able to help partially cover page charges (possibly up to a few thousand dollars) in case there is a need. When the paper is accepted, Olivia will ask the publisher to work with Christian and Paul to have their organizations settle the invoice for the page charges. Submission of the manuscript is expected within the next week. Olivia will contact the special issue guest editor Joshua Fu ahead of time to alert him of the pending submission.

Following the presentation by Anam Khan and Olivia regarding their planned work on comparing stomatal ozone deposition across models and deriving observation-based constraints during the February call, Christian had asked all groups contributing simulations to the Activity 2 overview manuscript the following questions:

- Q1: If needed, would you be interested in contributing additional simulations to this follow-up work?

- Q2: Do you have a constraint on how many such sensitivity simulations you might be able to perform, and during which timeframe you could perform them?

- Q3: Are you planning to propose and lead any follow-on work, either using the exiting observational datasets and model simulations, or additional model simulations?

- Q4: If so, when could you propose your planned activity to all participants during one of our regular calls, so that we can continue to coordinate planned activities?

The following feedback was received by email prior to the call, during the call, and by email after the call:

	Q1	Q2	Q3	Q4
Paul	Sure. One caveat – I might want to do more than one version of the	Depends on how many you are thinking (i.e. if you want to do	(also see below) Yes, there's a couple of ideas	(also see below) Next meeting (Tuesday) would

	ECCC models! e.g. with a more recent version of the ECCC contribution(s) in addition to the original(s) in the initial paper led by Olivia. I'm getting better comparisons to the obs with a revised version of the GEM-MACH-Wesely approach, for example, and was thinking I'd have another look at Leiming's code.	1E6 perturbations, delivered tomorrow, maybe not – but 10's to maybe 100 over a month, where the inputs are formatted the same as our current inputs, sure). So…over what timeframe? The code chugs through one run for all eight sites in about a minute or so, FYI. Assuming that the inputs are defined as individual input datasets that are otherwise formatted like the existing ones (I'm assuming that's what would be provided for input, here), chugging through a large number is now relatively easy – modify the script that runs them, and chug through a larger number. So the key thing would be to define the scenarios as separate input files (as opposed to needing more mods in the models for each scenario); if that's how it's done, the overhead to do	we'd (fellow ECCC scientist Colin Lee and myself) would like to pursue & lead, see attached description, assuming folks are interested. Use of different machine-learning techniques to identify input conditions leading to poor fits between point model and obs, and to determine constraints on the coefficients used in each model's equations that might improve the fit with obs using machine learning.	work for both of us to go over the two ideas; we'd need 10 minutes or so (we'll just put the Word file up on the screen and go over same). You could circulate the attached Word file around to the larger group a priori if you want, or I could (let me know).

		more is pretty small.		
Laurens	sure, e.g. doing the simulations with or without the soil moisture limitation but also, already done before, exlcuding the role of in-canopy chemistry	with the set-up I can very easily do extra simulations. Redoing the model runs for the 5 forest sites with the modified input files generally took me some 1-2 hours of work	We have the MSc thesis project on diagnosing the impact of the soil hydrology on the simulated Vd/FO3 for some of the forest sites (initially focussing on Borden) … Might pick up some of the work myself being ready with most of the teaching being done halfway April.	Can present some of this also when I know that we will make much faster progress, April/May?
Lisa	Yes (hopfully would be quicker now the model is set up!)	Easier to do over the summer (i.e. not between Oct and March)	No	No
Jon	Likely yes, need to check with Limei	Need to check with Limei	No	No
Jesse	Yes	No significant constraints were mentioned	Currently using observational datasets to optimize selected STAGE parameters – no analysis of other models	Not discussed
Johannes	Yes	No significant constraints were mentioned	No	No
Roberto	Yes	No significant constraints were mentioned	No	No

Paul and Colin presented the following two follow-up projects they intend to pursue. This information was also circulated to all call participants just prior to the call.

Two proposed projects for AQMEII4 continued point model comparisons, both involving techniques of machine learning to analyze the deposition data and point model output, both to take place concurrently starting in April. Colin Lee, Paul Makar (ECCC), March 3, 2023.

(1) **Hierarchical clustering analysis of point model deposition:** Using a hierarchical clustering code developed by Colin Lee et al (ECCC), we would like to investigate and hopefully determine the meteorological conditions resulting in poor model performance, for the suite of point models. The conditions under which a given model performs poorly may be in common with other models or be idiosyncratic to that model. The basic idea: The meteorological data for which observed deposition velocities are available will be paired with time series of the differences between modelled and observed deposition velocity from each model, as well as the time series of relative differences (+/-%). The hierarchical clustering code will be used to analyse the meteorological time series: clusters will be generated using a (1-R) metric, where R is the Pearson correlation coefficient. The clustering thus groups highly correlated meteorological records together. The time series of the clusters will then be compared to the time series of model performance: the aim is to see if specific meteorological clusters pair well with poor (or good!) model performance relative to the observations. This in turn would help identify the conditions under which individual models perform poorly or well, potentially providing information on the causes of poor or good model performance. The extent to which the same clusters are associated with poor or good model performance across models will help determine whether the underlying causes are common to the suite of models, or specific to a particular model. What would be required here is just the model time series for each model, and would be open to anyone interested in participating (including new/improved models coming on-line subsequent to the initial Activity 2 overview paper). References: Soares et al (ACP, 2018), Solazzo et al (Atm Env, 2012).

(2) Machine learning to improve gas-phase deposition algorithms: There are a number of machine learning tools available such as random forests and deep learning which could be brought to bear on this data set. The techniques all have a similar foundation, which is finding a set of coefficients or logical splits for the input variables that creates a prediction of the output variable that best matches the set of observations. These methods have shown very promising results in many applications in the air quality field. I (Colin) would like to try several techniques on the available deposition velocity observation data set. Firstly, this will involve just training a few different machine learning models using the meteorological and land-use variables as input to predict the deposition velocity. These models tend to provide efficient, accurate systems that can replace existing parametrizations in models, although the ease of gaining any physical insights from these models can vary. A more recent development is the idea of Physics Informed machine learning where you provide mathematical constraints on the system you're training. This makes physical interpretability much easier, although sometimes at the expense of model accuracy. The mathematical constraints in this case would be the form of the deposition velocity equations used in the model (the resistance network). Given that there are multiple physical forms of the deposition algorithms, we could gain insight into the resistance levels in each model that result in the closest match to observed deposition velocities. Finally, we can vary the subsets (ie, leave out a few weeks from each site, or a whole site) of the input data used to see how general any of the above models is – if the results from the training on subsets of data match the results on the whole dataset, we can be more confident that such a model is fairly general. If leaving out data results in different coefficients, that implies that we are overfitting the data and that we are very sensitive to the model structure. The data required would be the timeseries of observed deposition fluxes and meteorological and land-use data at each site, and the algorithms (or code, if available) for the deposition algorithms to be investigated.

Following the presentation of this proposed work by Paul and Colin, several call participants offered feedback and suggestions for their considerations. Paul and Colin noted these suggestions.

Johannes made the suggestion that in the next phase we should focus on model biases caused by key parameters rather than focusing on meteorology-driven model variability, because key parameters might be driving the largest model differences.

Jesse noted that the work suggested by Paul and Colin nicely complements his work using STAGE, which he is writing up right now for the special issue and will present on at ITM.

The next call is currently scheduled for Tuesday April 4, 2023 at 10:00 EDST / 14:00 GMT / 15:00 BST / 16:00 CEST. If there is a change in schedule, an updated calendar invitation will be sent to all participants.