AQMEII4 FAQ, version 4 (January 16, 2020)

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1) Q: Our model runs start on January 1, but we need to start our model 2 weeks to 1 month before that time, in order to allow for spin-up. What emissions do we use for that December spin-up period? Similarly, what should we use for chemical lateral boundary conditions?
   A: Our recommendation is to use the given year's emissions for December. i.e. for a 2009 year simulation, use the December 2009 emissions for the spin up period in December of 2008; for a 2016 year simulation, use the December 2016 emissions for the spin-up period in December of 2015. With regards to the chemical lateral boundary conditions, Christian has contacted ECMWF and they will be able to provide fields to generate the lateral boundary conditions for the spin-up periods in December.

2) Q: In the past, AQMEII recommended that the ECMWF reanalysis values for sea-salt should NOT be used. Has that changed?
   A: Two important considerations with regards to the ECMWF particulate matter boundary conditions arose during the Hamburg meeting. These are further documented at https://confluence.ecmwf.int/display/CKB/CAMS+global+sea+salt+aerosol+mixing+ratios
   a. The sizes specified in the ECMWF information are in radius, not diameter – this needs to be taken into account when transferring the ECMWF particle speciation to the participant model speciation. Furthermore, as documented in the second paragraph of the URL provided above, for sea salt these radii are specified for wet aerosols at an ambient relative humidity of 80%. To calculate the dry radii, the nominal radii of the sea salt bin limits (0.03, 0.5, 5 and 20 microns) should be divided by a reduction factor of 1.99.
   b. The mass reported by ECMWF as sea salt mass is the wet aerosol mass. In order to determine the corresponding dry sea-salt mass, the ECMWF values need to be divided by a factor of 4.3.

   Given the above considerations, we are recommending that participants use the ECMWF CAMS reanalysis data, including the sea-salt values, for their boundary conditions.

3) Q: How do we map from our own model's land use categories to the AQMEII-4 categories? We are not expected to run our models with the AQMEII-4 categories, are we?
   A: Participants should run with their own "native" land use categories! The transformation to the AQMEII-4 land use categories should happen as part of the post-processing. Participants will need to construct the mapping between their land use categories and the AQMEII-4 categories, then create land-area-fraction weighted values for reporting, in the AQMEII-4 categories. For example, for the resistance quantity R, the contribution of the native land-use categories i to AQMEII-4 category j at grid-cell x,y can be represented by the following equation:

$$R_j(x,y) = \sum_{i \in j} \left\{ \frac{A_i(x,y)}{\sum_{i \in j} A_i(x,y)} \, R_i(x,y) \right\}$$

That is, the user must determine which of the native land use categories i contribute to AQMEII4 land use category j (i.e sums over all i which contribute to j in the above equation, then use the native land use mode area fractions Ai to determine the fractional contribution of the I'th land use category to the j'th AQMEII-4 category, locally for each grid-cell on the AQMEII-4 destination grid and at the station locations. The reported values are thus area-weighted according to the contributions of the native land use categories to the AQMEII-4 categories, at each grid cell.

4) Q: We understand that our models are to be run using their native land use categories, and the results are to be mapped by area fraction into the 16 AQMEII4 land use categories. However, what do we do if there is no contribution to an AQMEII4 category from the model's own land use category?
A: The value in that case should be reported using the "no data" code, -9.0. We note that different participants will be using different sources of land use data, and as a result, the location and relative fraction of the AQMEII-4 land use categories may vary between participants. However, both the native land use categories and resulting AQMEII-4 land use categories are to be reported in gridded form by each participant, which will help determine the extent of overlap and the regions of the grid that are most suitable for direct comparison, and part of what the reporting will determine is the extent to which differences in deposition relate to differences in the underlying land use databases.

5) Q: Our model domain extends beyond the boundaries of the region defined for emissions by AQMEII-4. What should we use outside of the defined region?
A: We leave this choice up to the participant. We note that this can introduce an additional source of uncertainty in the model intercomparison.

6) Q: Our model has the capability to calculate lightning emissions inline. Can we use these model calculated lightning emissions instead of the GEIA-based climatological lightning emissions distributed to all participants?
A: We strongly encourage the use of the common emission dataset. The use of model calculated lightning emissions could be an interesting sensitivity study some groups may wish to perform. For the vertical allocation of the GEIA emissions, please use the "midlatitude" reference profile contained in the "README_Lightning" document posted along with the emissions at https://drive.google.com/drive/folders/1R83HYZgn6qd0L01UN_u5nHeQ5swbMCYj. The profile contains fractional allocations in 1 km increments, it is recommended to uniformly split emissions across multiple model layers that may occur in a given 1 km increment and aggregate emissions if a given vertical layer is thicker than 1 km. We also encourage the sharing of code for the preparation of model-ready lightning emission files between groups using the same model.

7) Q: The units for which deposition fluxes should be reported as eq ha-1 for some species and g ha-1 for others. Can you elaborate?

A: For wet and dry flux variables contributing to acid deposition (WFLUX-HSO3-, WFLUX-SO4=, WFLUX-NO3-, WFLUX-NH4+, WFLUX-BCT1, DFLUX-SO2, DFLUX-NO2, DFLUX-NO, DFLUX-HNO3, DFLUX-NH3, DFLUX-PAN, DFLUX-HNO4, DFLUX-N2O5, DFLUX-ONIT, DFLUX-P-SO4, DFLUX-P-NO3, DFLUX-P-NH4, DFLUX-P-BCT1, BFLUX-P-BCT2, and DFLUX-HONO), the deposition fluxes should be reported in units of eq ha-1. For all other variables, units of g ha-1 should be used except for DFLUX-P-SS where units of moles ha-1 should be used.

To convert fluxes from g ha-1 to eq ha-1, the mass flux has to be converted to a molar flux of S or N using the molecular weight of the species and the number of S or N in that species and then be multiplied by the valency of the ion (e.g. 2 for SO4, 1 for NO3, NH4, etc.). For example, to convert dry deposition fluxes of SO_2 from g ha-1 to eq ha-1, they are first converted to units of moles S ha-1 by dividing the mass flux by 64.0588 (to convert g of SO_2 to moles of S), and then multiply by 2 (i.e. assume a charge of -2 for each mole of S). Similarly, all of the nitrogen gases need to be converted to moles N ha-1 and a charge of -1 is assumed (no need to multiply by 1). The rationale underlying these calculations is that the sulfur deposition is assumed to eventually result in sulfate formation, and the nitrogen deposition is assumed to eventually result in nitrate formation. Equivalents per unit area per unit time are the units used to calculate critical load exceedances.