AQMEII4 Errata, Corrections, and FAQ, version 6 (November 11, 2020)

P.A. Makar, based on notes taken from the September 24th 2019 meeting in Hamburg.
C. Hogrefe, based on notes taken during the October 10th 2019 conference call
C. Hogrefe, based on email correspondence with R. Kouznetsov (FMI)
C. Hogrefe, based on email correspondence with P.A. Makar during December 2019 and January 2020
C. Hogrefe, based on email correspondence with P.A. Makar during January – February 2020
C. Hogrefe, based on email correspondence with P.A. Makar during October - November 2020

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.

However, the land use weighting should be used differently, depending on the field being reported. Three examples follow:
For resistance fields, the weighting is applied to the inverse of the resistances. 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:

$$\left(R_j(x,y)\right)^{-1} = \sum_{i \in j} \left\{ \frac{A_i(x,y)}{\sum_{i \in j} A_i(x,y)} \left(R_i(x,y)\right)^{-1} \right\}$$

For the land-use-specific deposition velocities (Vd), and the conductances (C), the area weighting is applied directly:

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

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

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.
We acknowledge that these are diagnostics – the different deposition modules may make use of the resistance and conductance terms in a fashion other than the area weighting shown. Nevertheless, this allows a comparison of the relative magnitude of different components going into the deposition calculations, across different models, hence helping in the analysis of the possible causes of differences between the different models deposition velocity values.

A similar issue arises when determining the "net" components for a given grid cell (see FAQ 10, below).

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.

8) Q: How are the "net" dry deposition parameters (e.g. VD-SO2, RES-SURF-SO2, etc.) different from the land-use specific parameters (e.g. VD-SO2-01, RES-SURF-SO2-01, etc.)?
A: There are two parts to the answer for this question.
First, for the deposition velocity itself (VD-SO2, and similar terms), the net deposition velocity is the deposition velocity *actually used by the model for that gas*; the final result of however the model puts together the deposition velocity to be used for that gas in each grid cell.
Second, for the other terms (resistances, conductances), they are to be the land-use weighted values of the terms calculated for the individual native land use types. We note that these only provide an approximation of how the land-use specific terms are used in deposition calculations, but are nevertheless useful to determine the relative importance of the different deposition pathways.
So, the "net" values are the native land-use weighted values consistent with a land-use weighted net deposition velocity. That is, using Wesely's model as an example, and Li as the land-use fraction of the i'th native land-use type, the net resistances and conductances for a grid-cell containing two native land use types are given below:

$$RES\_SURF_{net} = r_{c,net} = \left(L_1 {r_{c,1}}^{-1} + L_2 {r_{c,2}}^{-1}\right)^{-1} = \left(\sum_{i=1}^{N} L_i {r_{c,i}}^{-1}\right)^{-1}$$

$$RES\_STOM_{net} = r_{s,net} = \left(L_1 {r_{s,1}}^{-1} + L_2 {r_{s,2}}^{-1}\right)^{-1} = \left(\sum_{i=1}^{N} L_i {r_{s,i}}^{-1}\right)^{-1}$$

$$RES\_MESO_{net} = r_{m,net} = \left(L_1 {r_{m,1}}^{-1} + L_2 {r_{m,2}}^{-1}\right)^{-1} = \left(\sum_{i=1}^{N} L_i {r_{m,i}}^{-1}\right)^{-1}$$

$$RES\_CUT_{net} = r_{lu,net} = \left(L_1 {r_{lu,1}}^{-1} + L_2 {r_{lu,2}}^{-1}\right)^{-1} = \left(\sum_{i=1}^{N} L_i {r_{lu,i}}^{-1}\right)^{-1}$$

$$RES\_CONV_{net} = r_{dc,net} = \left(L_1 {r_{dc,1}}^{-1} + L_2 {r_{dc,2}}^{-1}\right)^{-1} = \left(\sum_{i=1}^{N} L_i {r_{dc,i}}^{-1}\right)^{-1}$$

$$\boldsymbol{ECOND\_ST_{net}} = \sum_{i=1}^{N} \boldsymbol{L_i} \left(\frac{\left(\boldsymbol{r_{s,i}} + \boldsymbol{r_{m,i}}\right)^{-1}}{\left(\boldsymbol{r_{s,i}} + \boldsymbol{r_{m,i}}\right)^{-1} + \left(\boldsymbol{r_{lu,i}}\right)^{-1} + \left(\boldsymbol{r_{dc,i}} + \boldsymbol{r_{cl,i}}\right)^{-1} + \left(\boldsymbol{r_{ac,i}} + \boldsymbol{r_{gs,i}}\right)^{-1}} \right) \boldsymbol{v_{d,i}}$$

$$\boldsymbol{ECOND\_CUT_{net}} = \sum_{i=1}^{N} \boldsymbol{L_i} \left(\frac{\left(\boldsymbol{r_{lu,i}}\right)^{-1}}{\left(\boldsymbol{r_{s,i}} + \boldsymbol{r_{m,i}}\right)^{-1} + \left(\boldsymbol{r_{lu,i}}\right)^{-1} + \left(\boldsymbol{r_{dc,i}} + \boldsymbol{r_{cl,i}}\right)^{-1} + \left(\boldsymbol{r_{ac,i}} + \boldsymbol{r_{gs,i}}\right)^{-1}} \right) \boldsymbol{v_{d,i}}$$

$$\boldsymbol{ECOND\_SOIL_{net}} = \sum_{i=1}^{N} \boldsymbol{L_i} \left(\frac{\left(\boldsymbol{r_{ac,i}} + \boldsymbol{r_{gs,i}}\right)^{-1}}{\left(\boldsymbol{r_{s,i}} + \boldsymbol{r_{m,i}}\right)^{-1} + \left(\boldsymbol{r_{lu,i}}\right)^{-1} + \left(\boldsymbol{r_{dc,i}} + \boldsymbol{r_{cl,i}}\right)^{-1} + \left(\boldsymbol{r_{ac,i}} + \boldsymbol{r_{gs,i}}\right)^{-1}} \right) \boldsymbol{v_{d,i}}$$

$$\boldsymbol{ECOND\_LCAN_{net}} = \sum_{i=1}^{N} \boldsymbol{L_i} \left(\frac{\left(\boldsymbol{r_{dc,i}} + \boldsymbol{r_{cl,i}}\right)^{-1}}{\left(\boldsymbol{r_{s,i}} + \boldsymbol{r_{m,i}}\right)^{-1} + \left(\boldsymbol{r_{lu,i}}\right)^{-1} + \left(\boldsymbol{r_{dc,i}} + \boldsymbol{r_{cl,i}}\right)^{-1} + \left(\boldsymbol{r_{ac,i}} + \boldsymbol{r_{gs,i}}\right)^{-1}} \right) \boldsymbol{v_{d,i}}$$

So, in short, the net deposition velocity is the net value used by the model, and the net values of the resistances and conductances are the native land-use-area-weighted values of the land-use-specific values for these terms.[1]

9) Q: The variable description for RES-SURF-SO2 in 0246-012 says "Net Surface Resistance", but in the LU-specific parameter tables (e.g. 0246-192 for LU Type 4), RES-SURF-SO2-04 is described as "AQMEII4 Land Type 04 Canopy Resistance". Can you please clarify?
A: The 'Net Surface Resistance' of TSDs 0241/0246-012 through TSD 0241/0246-122 is the same variable described as the land-use-specific 'Canopy Resistance' of TSDs 0241/0246-0132 through 0241/0246-442: both refer to the "r_c" term, the total resistance due to vegetation in the deposition velocity equations in the guidance document.

10) Q: Some of the TSDs are asking for total Leaf Area Index (LAI-T) to be reported. Some modeling systems use different representations of Leaf Area Index in different portions of the code (e.g. biogenic emissions vs. deposition). Which Leaf Area Index should be reported in the cases?
A: Please report the Leaf Area Index that is specifically being used in your dry deposition calculations. Note that some deposition modules make use of a lookup table, assigning leaf area index by land use type for a given season or month: for these modules, *the land-use-type weighted* leaf area index should be reported; the lookup table values are multiplied by the land

[1] An example illustrating the difficulty in defining "net" resistances which are consistent with the use of land-use specific resistances, when the deposition model combines land-use weighted deposition velocities to calculate the net deposition velocity in each grid cell, is as follows, again using Wesely's model: Suppose a grid cell contains only two land use types, with land use fractions L_1 and L_2. If the quasi-laminar sublayer resistance and the aerodynamic resistance are the same for both land use types, then the net deposition velocity for the grid cell, using the usual land use weighting of land-use-type specific deposition velocities, will be:

$$v_d = L_1 v_{d,1} + L_2 v_{d,2} = \frac{L_1}{r_a + r_b + r_{c,1}} + \frac{L_2}{r_a + r_b + r_{c,2}}$$

In the above case, deposition velocities $v_{d,1}$ and $v_{d,2}$ are the deposition velocities for land use types 1 and 2 respectively. These have "net surface" aka "net canopy" resistances of $r_{c,1}$ and $r_{c,2}$, respectively. One could also define a net surface or canopy resistance in one of two ways. One could, for example, define the net canopy resistance from the deposition velocity equation:

$$v_d = \frac{1}{r_a + r_b + r_{c,net}}$$

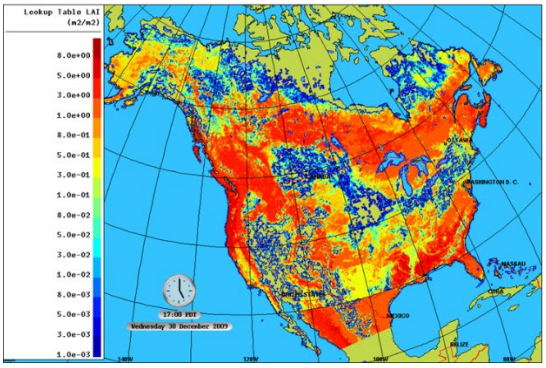
Combining this with the equation above gives the following formula for $r_{c,net}$:

$$r_{c,net} = \left(\frac{L_1}{r_a + r_b + r_{c,1}} + \frac{L_2}{r_a + r_b + r_{c,2}} \right)^{-1} - r_a - r_b$$

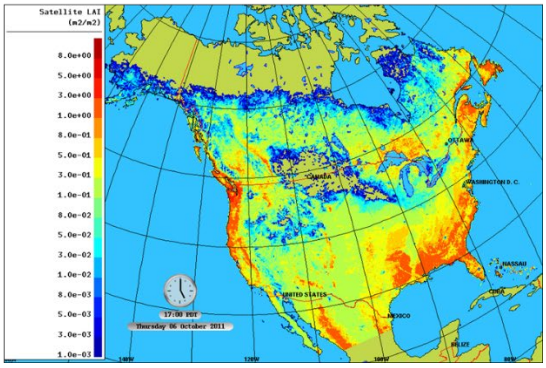
While this is relatively easy to do for the net surface or canopy resistance, the determination of net values of the *components* of $r_{c,net}$, and the conductances, can be difficult, when the land-use area weighting is applied to the deposition velocities and not the components, in the deposition module.

use type fractional area within each grid cell, and the sum is reported. Note that these may be very different from more recent sources of LAI data such as MODIS (see example, below, and note https://agupubs.onlinelibrary.wiley.com/doi/full/10.1002/2015JD024406).

Lookup table



December MODIS Values



11) Q: Some of the TSDs are asking for Aerosol Optical Depth (AOD) values to be reported. Is there any filtering to be applied prior to output to remove in-cloud enhancement of particle AOD?
A: No. As a result, the maximum AOD's generated by the models may be much higher than observed by satellites. Satellite AOD retrieval algorithms filter out cloudy regions by either assuming an upper limit on the AOD or by making use of other retrieved information. The models may have aerosols within clouds or very high relative humidity regions which are very large, yet are not necessarily considered to be cloud droplets – with resulting large values of AOD. A comparison of AQMEII-4 reported model values to satellite observations may thus require some post-processing of the model fields, e.g. eliminating all cells with relative humidities above 99%.

12) Q: Reporting of dry deposition parameters for LU category 1 (water)?
A: All the relevant parameters are to be reported (those which feature in the water deposition calculation). For those which are not relevant (e.g. terms not used in the water dry deposition equation), the "missing" code (usually -9) should be used.

13) Q: The gridded TSDs for sequences *-001 request emissions for E_PM2_5 (Accumulated emission of primary PM2.5) and E_PM10 (Accumulated emission of primary PM10), and also request E_WBDUST (Accumulated emission of Wind Blown Dust (all particle sizes)) and E_SS (Accumulated emission of Sea Salt (all particle sizes)). Should E_WBDUST and E_SS be included in E_PM2_5 and E_PM10 or not?
A: E_WBDUST and E_SS should NOT be included in E_PM2_5 and E_PM10. Emissions of wind-blown dust and sea-salt are recognized as model-specific parameterizations, as opposed to AQMEII4 specified emissions – consequently, they have been split off from the total PM emissions so that these model-dependent differences can be examined.

14) Q: The TSDs for sequences *-005 request variables WETCAN ("Canopy wetness, 0.0 if dry and 1.0 if wet") and FWET ("Wet Surface, unitless fraction"). Can you elaborate on the differences?
A: Generally, participant will report values for just one of these two variables while reporting missing values ("-9") for the other, depending on their dry deposition scheme. Some models have a binary switch for whether or not a surface is being treated as dry or wet (with a variety of criteria for making that choice), and some make use of sliding scale. WETCAN is used for cases in which a binary switch is used while WETCAN can be used by schemes who define a fractional wetness. Put differently, some models will report WETCAN values of 0 or 1 and FWET values set to the no data code, while others will have WETCAN set to -9 and use FWET to report the fractional wetness value.

15) Q: The TSDs and src and cf metafiles shared on October 8, 2020 list the units for DFLX-*-O3, DFLX-*-H2O2, and DLFX-*-HCHO in sequences -102, 112, and 122 as "eq ha-1". Shouldn't these be "g ha-1" rather than "eq ha-1" since the DFLUX-* variables for these three species in -002 also are in "g ha-1"?
A: Yes, this was a typo in that version of the TSDs and src and cf metafiles that will be corrected in a future update. If you are already working on postprocessing these sequences, please use "g ha-1" when preparing data for DFLX-*O3, DFLX-*-H2O2, and DLFX-*-HCHO and edit the src metafiles to correct the units for these variables prior to running enform_aq.