Participant Call June 2, 2022

Participants: Christian Hogrefe, Holly Nowell, Jesse Bash, Donna Schwede, Paul Makar, Roberto San Jose, Rohit Mathur, Jon Pleim, Ummugulsum Alyuz

Grid intercomparison (Activity 1)

- Participant updates on reruns, postprocessing, data upload, and analysis. **See attached table for summary of updates below.**

  - Paul: All reruns are completed, .ens files for last year will be uploaded tomorrow. In July, will move on to analysis of GEM-MACH runs, then later on critical load analysis.
    - Which model runs are still in flux for deposition fields? Christian will provide update via email.
  - Roberto:
    - NA2016: uploaded re-processed resistances (now inverted) for NA2016. Used MIN_POS of 1E-24 so some low resistances (e.g. RES-MESO-HNO3-*) exceeded the enform format specifications when inverted. Will reprocess with MIN_POS set to 1E-08 and re-upload by middle of June
    - Then will reprocess resistances for EU cases - ~1 month
    - NA2010 simulations are ongoing but had to be paused due to the computer getting too warm. Currently completed through the end of September. Hope to finish runs by the end of June. Then will take 1-2 months for post-processing and upload
  - Christian: CMAQ STAGE reruns completed, postprocessing to be completed this week, uploads of gridded data and receptor extractions next week
  - Ummugulsum: Restarted runs, 2010 currently running, almost completed. Also post-processing old 2009 runs to get a feel for model outputs. Post-processing scripts are still running. Next week 2010 CMAQ runs should be completed, then 1-2 weeks for 2010 rerun post-processing. Still likely going to re-run 2009 as well.
  - Holly: Started 2010 GEOS-Chem runs, so far things are looking o.k., so hopefully will start 2016 soon. Estimate several months before post-processed data becomes available.

Point intercomparison (Activity 2)

- Participant call held May 24, focused on updated input datasets
  - Prescribed parameters like surface roughness, fixed time zone issues, screened for and removed outliers, consistently estimated leaf wetness when not available.
  - See attached power point presentation for details.

- Revised input datasets for all sites except Auchencorth Moss and Easter Bush distributed to modelers on May 24 – please see Olivia's email below.

Subject	**New AQMEII4 Activity 2 forcing files**
From	Olivia Clifton

To	
Cc	Schwede, Donna
Sent	Tuesday, May 24, 2022 7:45 PM

Hi all,
Please find the new forcing data in AQMEII/Flux Datasets/*site* on GoAnywhere
This directory contains:
1. *dataset csv file*
2. *metadata documentation*
    a. *see here for parameter definitions, descriptions of & units on variables (& how to use them)*
3. *pdf of time series plots of all variables in dataset*
4. *directory of processing scripts*
5. *directory of raw data*
6. *[site dependent] directory of literature/notes from PIs*

you should not need to access 4-5, and not really 6 (hopefully the metadata plus my draft paper has extracted the relevant info, at least for this stage); 3 is just to help you, if you see anomalous values in your modeled deposition velocities then this could help you figure out what is going on

1-4 are missing for Easter and Auchencorth - we are on this.

Please find the new Fortran wrapper code and script has been uploaded to AQMEII/Fortran Wrapper and Script on GoAnywhere

There are large changes to the driving datasets, so your old fortran wrappers will not work.

Please load your model results to AQMEII/Single Point Model Results/*version of your model* on GoAnywhere asap

Additional notes
> · *Please use LULC type, soil parameters (field capacity, wilting point, and saturation values both for volumetric soil moisture and water potential), & reference height as defined in the metadata*
>> o *The B variable for soil (slope of the saturation - matric potential line) should probably be used by TEMIR, STAGE, M3-Dry, MLC-Chem and ECCC Zhang*
> · *Leaf wetness*
>> o *Sometimes given as 0 or 1, sometimes fractional (it says which one for each site in the metadata)*
>> o *Please use our indicators of leaf wetness (except WRF-Chem + TEMIR Zhang (& possibly ECCC Zhang) who indicate leaf wetness with precipitation).*

· Please see which soil moisture and soil temperature variables you should use for surface vs. root zone in the metadata
· Please use roughness height, displacement height, and solar zenith angle from the driving dataset - do not calculate your own
> *o Following the discussion today on whether we should incorporate displacement heights into Ra equations coming from grid scale models. If you want to include displacement height in Ra & edit your Ra equation, just let me know; we would encourage you to do so.*

· For models that only need an indicator of whether there is snow, please define the presence of snow as snow depth > 1 cm. There is no snow if snow depth is <= 1 cm, or if snow is missing (whether for the entire dataset or whether within a dataset that generally has snow depth).
· If you see strange values in the forcing data, please do not screen them out yourself, or fill them with something else. Please let us know and we will figure out what to do.

- Hope to circulate the remaining two datasets soon.
- Ask modelers to upload results at their earliest convenience and keep Olivia informed about progress and timelines
    - Roberto: running with new input data, expect to finish in 1-2 weeks
    - Paul: Philip will get started on this after finishing the grid model processing. Hope to start running by end of July
    - Jon: hasn't started to use the new data yet.

- TOAR deposition work group to AQMEII4 participants: Olivia, Donna, Stefano and Christian will have a follow-up call with Leiming Zhang and Lisa Emberson, stay tuned.

Special issue

- In June, Stefano and Christian will reach out to Copernicus and Joshua to extend the special issue by either a year (August 2023) or end of 2023.

HTAP workshop - Olivia presented an AQMEII4 overview on May 19

Next call: July 14, 9:00 EDST / 15:00 CEST

Upload Status June 2, 2022.

	Continent / Year	001 (gases + aerosols)	002 (grid-scale wet and dry dep fluxes)	005 (meteorology)	012 – 122 (grid-scale dry dep diagnostics	132 -442 (LU-specific dry dep diagnostics)	452 (NH3 bi-directional)	462 (AQMEII4 LU fractions)	472 (native LU fractions)
10700 (EPA CMAQ M3DRY)	NA 2010	x	x	x	x	x	x	x	x
	NA 2016	x	x	x	x	x	x	x	x
10701 (EPA CMAQ STAGE)	NA 2010	x	x	x	x	x	x	x	x
	NA 2016	x	x	x	x	x	x	x	x
10702 (IASS WRF-Chem)	EU 2009	x	x	x	x	x		x	x
	EU 2010	x	x	x	x	x			
	NA 2010	x	x	x	x	x		x	x
	NA 2016	x	x	x	x	x		x	x
10703 (ECCC GEM-MACH BASE)	NA 2010	x	x	x	x	x	x	x	x
	NA 2016	x	x	x	x	x	x	x	x
10704 (ECCC GEM-MACH ZHANG)	NA 2010	x	x	x	x	x	x	x	x
	NA 2016	x	x	x	x	x	x	x	x
10705 (ECCC GEM-MACH OPS)	NA 2010	x	x	x	x	x		x	x
	NA 2016	x	x	x	x	x		x	x
10706 (TROPOS COSMO-MUSCAT)	EU 2009	x	x						
	EU 2010	x	x						
10707 (TNO LOTOS-EUROS)	EU 2009	x	x	x	x	x		x	
	EU 2010	x	x	x	x	x		x	
10708 (UPM WRF-Chem)	EU 2009	x	x	x	x	x		x	x
	EU 2010	x	x	x	x	x		x	x
	NA2010								
	NA 2016	x	x	x	x	x		x	x
10709 (UCAR WRF-Chem)	NA 2010	x	x	x	x	x		x	x
	NA 2016	x	x	x	x	x		x	x
10710 Hertfordshire CMAQ	EU 2009								
	EU2010								
10711 Hertfordshire WRF-Chem	EU2009								
	EU2010								
10712 FSU GeosChem	NA 2010								
	NA 2016								

Notes:

- 10701 (EPA CMAQ STAGE) reruns completed, upload of .ens files expected by 6/10/2022
- 10702 (IASS WRF-Chem) questionable values in wet deposition fields for NA2010, NA2016, and EU2010. No recent updates from Aura regarding potential updates to these fields
- 10703 (ECCC GEM-MACH) reruns completed, uploaded of NA2010 .ens files expected by 6/3/2022
- 10706 (TROPOS COSMO-MUSCAT) – uploaded partial fields are bad, no recent updates on potential new model simulations. Drop model from analysis
- 10707 (TNO LOTOS EUROS) questionable values for some LU-specific deposition diagnostics, Richard is investigating, no updates since early May
- 10708 (UPM WRF-Chem)
  - reprocessing diagnostic resistances for NA2016, EU2009, and EU2010, expect to upload revised files by middle of July
  - performing simulations for NA2010 (not originally planned). Expect to upload results by end of August
- 10710 (Hertfordshire CMAQ STAGE) close to finishing EU2010 reruns and uploading post-processed outputs from old EU2009 runs for screening purposes. Likely will rerun EU2009 after finishing EU2010 reruns. If not rerunning EU2009, the post-processed outputs from the old EU2009 runs are for screening purposes only (to identify issues with post-processing) but should not be used in publications.
- 10711 (Hertfordshire WRF-Chem) runs not initiated and no longer expected.
- 10712 (FSU GEOS-Chem) – running NA2010, plan to start NA2016 soon. Expects that it'll be several months before data will be uploaded, i.e. late August.

Until further notice: browse and download uploaded files and receptor extractions at https://ensemble.jrc.ec.europa.eu/ensemble/pvt/aqmeii4/ - no login required

AQMEII Activity 2 Updates

May 24, 2022

Input Data Updates

- Goals
  - Have inputs be consistent from site to site
  - run each of the models with a consistent set of inputs
- Single metadata file for each site
  - List of variables and units as found in the files
  - Data policy information
  - Summary of R script processing
- Combine R scripts for data processing and AQMEII flagging
- Updated wrapper

Input Data Updates (cont)

- All sites
  - Define field capacity and wilting point
  - Define land use type
  - Define reference height
  - Provide surface roughness and displacement height as in Meyers et al (1998)
    - Special case for LAI < 1 was not used
  - Fill CO_2 values
  - Provide solar zenith angle
  - Drop unneeded data/columns (e.g. snow cover)
  - Additional QA/screening
  - All precipitation is as a rate with units of mm/s
  - Leaf area is all single sided

Time reporting QA

- Chris Holmes used the zenith angle and solar radiation to identify some time reporting issues - we asked for local time
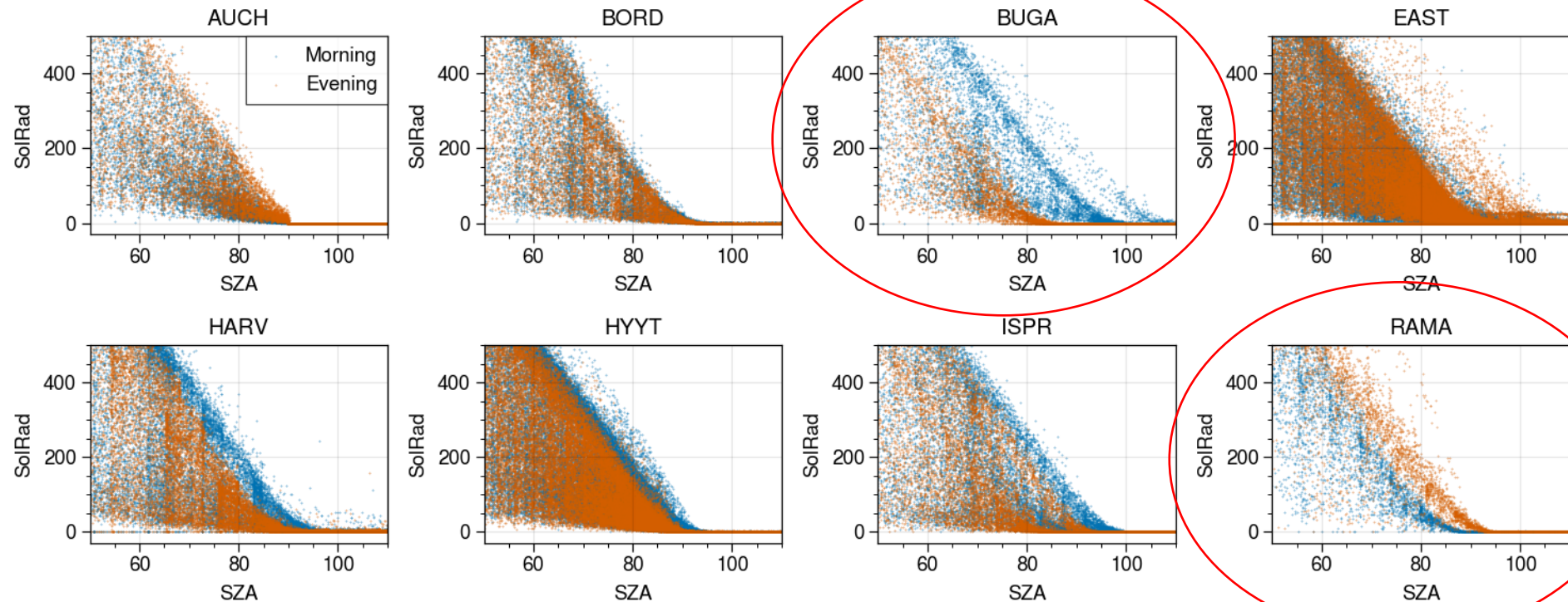
Additional radiation file was in UTC

Original Ramat file had some DST values

Auchencorth Moss

- Model as **wetland**
- Set odd ozone flux values (up to index 9000 / 7/6/2016) to NA
- Set odd PAR values (index values 33532-33533 11/29/2017 and 33621-33622 12/1/2017) to NA
- Set odd large negative Rnlite values (< - 50) to NA
- Set odd low CO_2 values (< 350) to NA
- **Divided LAI by 2** (original values are double sided, we want single sided)
- Set Wetness values > 0 to 1. (instrument cannot reliably provide fractional information)
- Change PAR unit string from "umol q m-2 s-1" to "umol m-2 s-1"

Borden Forest

- Fixed some date/time issues (hour ending vs hour beginning, 0-23 vs 1-24 hr clock, etc)

- Air temperature is now the temperature at the height of the sonic for consistency – not all models could or were using multiple temperatures

- Divided precip by 3600 to convert to mm/s

- Soil moisture and temperature processing for sites A and B done in R
  - 2 cm and 50 cm soil moisture
  - 5 cm and 50 cm soil temperature

Bugacpuszta

- Time shift for radiation as noted earlier
- **RH now a fraction** like other sites
- Convert 3 cm soil moisture from percentage to fraction
- Convert 30 cm soil moisture from percentage to fraction
- Cap relative humidity at 1
- Divide precipitation by 1800 to convert to mm/s
- Set 3cm soil moisture values < 0.02 to missing

Easter Bush

- Estimate of soil moisture is 40% - added this as a constant value based on discussions with M. Coyle
- Add radiation checks for negative values during day and positive ones at night
- Wind sectors excluded are 130-150 degN and 305-315 degN
    - there are some LAI values that are missing or 0 that correspond to excluded wind directions; set LAI=0 to missing
    - check for excluded wind directions - make sure o3 flux and vd are set to missing for the excluded directions;
    - also set ambient temperature to missing so that all models definitely won't run for the excluded directions
- Set odd Ta values (<-50.) to NA
- Set odd H values (abs(H) > 250) to NA
- Set Wetness values > 0 to 1. (instrument cannot reliably provide fractional information)
- Set odd Av_Soil_T (< -10. or > 25.) to NA
- Set odd low CO_2 values (< 300) to NA
- Cap relative humidity at 1
- Set continous period of 0.02 solar radiation values (index 168,700 - 182,200) to NA
- Set continous period of 0 / very small (<1) PAR at beginning of time series (index 1 - 11000) to NA
- **Divided LAI by 2** (original values are double sided, we want single sided)

Harvard Forest

- Replace filled wetness with the CMAQ/CASTNET equation
  - Dropped leaf_wetness; kept_leaf_wetness_filled
- Cap relative humidity at 1

Hyytiala

- Cap relative humidity at 1
- Set odd PAR value at index 1096 (1/23/2002) to NA
- Set odd CO2 values at index 69776 - 69808 (12/24/2005 15:40 to 12/25/2005 07:30) to NA
- Divide precipitation by 1800 to convert to mm/s
- Add CMAQ/CASTNET method leaf wetness calculation to fill sfcwet-sensor based values
- Replace sensor-based leaf wetness with CMAQ/CASTNET method after index 111,160 - 2008/5/4
- Fill in beginning of time series for soilm_A, soilm_B1, soilt_A, and soilt_B1 (through 1/12/2005 for soilm and through 1/1/2006 for soilt)
- Remove variables soilmoisture and sfcwet from output file
- Remove variable soilT from output file
- Changed **snow depth from cm to m**
- Changed PAR unit string from "umol q m-2 s-1" to "umol m-2 s-1"

Ispra

- Fill in missing LAI at the beginning of the period
- Replace constant LAI value of 3.603057 at end of time series (index 50022 - 52565, 2015/11/9 - 2015/12/31) with average day-of-year values
- Recalculate ozone deposition velocity as - flux / mixing ratio
- Cap relative humidity at 1
- Set odd large negative net_radiation (< -500) to NA
- Set odd large negative latent heat flux (< -200) to NA
- Add CMAQ method leaf wetness calculation to fill sensor based values
- Replace sensor-based leaf wetness with CMAQ method after index 39650 (2015/4/7)

Ramat Hanadiv

- Updated data with corrected time stamp
- **Convert relative humidity to fraction**
- Cap relative humidity at 1
- Set spurious large net_radiation values (< -250 W/m2) to NA
- Set spurious low CO2 values (< 150 ppm) to NA
- Divide precipitation by 1800 to convert to mm/s

Remaining Issues

- Auchencorth and Easter Bush
  - Deposition velocity and wind speed reported at 1 m
    - Calculated from the sonic amemometers windspeed and turbulence or interpolated from the windspeed gradient, corrected for stability
  - Friction velocity from sonic

- Fractional vs volumetric soil moisture
  - Sites seem to vary in what they are reporting
  - What do the models need?

- Sensible Heat flux – still spurious values (see example next slide)
  - Are the models using these in their calculations

H AuchencorthMoss