AQMEII4.A3 - Point Intercomparison of Dry Deposition Schemes - Overview

Similar to previous phases of AQMEII, participants in Phase 4 Activity 1 (AQMEII4.A1) will be running gridded air quality models for domains in Europe and North America with common inputs. We are also inviting participation in a point (i.e. box model or zero-dimensional) intercomparison of dry deposition schemes as part of AQMEII Phase 4 Activity 3 (AQMEII4.A3). Participants will be asked to calculate deposition velocity and its component resistances for a suite of gases and particles under prescribed surface and atmospheric conditions at specific sites. The goal is to reveal and understand the variation in dry deposition between multiple schemes under identical environmental conditions in the context of implications for air quality and ecosystems. This activity will aid the larger AQMEII4.A1 3-D model intercomparison in which models use model dependent surface and atmospheric conditions as well as different dry deposition schemes.

Science questions

- How much and why do current dry deposition schemes differ under identical environmental conditions?
  - Which processes (e.g. stomatal conductance, cuticle uptake, etc.) control the deposition velocity at individual sites and how variable are the processes among schemes?
  - What is the impact of the assumed land use or vegetation type on deposition velocity?
- How well do dry deposition schemes predict measured deposition velocity?
- How does the sensitivity of deposition velocity to individual environmental factors and surface conditions vary across dry deposition schemes?

Planned approach

Input data: Participants will be provided measurements of meteorology and ozone flux with hourly or half-hourly time resolution from long-term sites as well as site information such as land use type, leaf area index, and canopy height. These data should be used to drive dry deposition calculations. Table 1 lists the variables that will be provided. Data is not gap filled but is quality assured and outliers are flagged. For data sets that do not contain values for leaf wetness, an additional column has been added for a leaf wetness estimation where the leaf is considered wet if the relative humidity exceeds 85%. If your scheme requires additional input data, please contact the planning team and we will determine if the required parameters are available. Additional site specific data on vegetation and soil properties is in Table 4.

Control simulation: For the first part of this effort, participants should calculate deposition velocities with the site observations with their dry deposition schemes and submit the model data. Simulated deposition velocities and fluxes for O_3, SO_2, HNO_3, and aerosols (0.1 µm, 1µm and 10 µm diameter, densities of 1.0 g cm^{-3} and 2.2 g cm^{-3} for each diameter) are requested and will be used for scheme intercomparisons and sensitivity tests. Evaluation studies will only include O_3 because the flux measurements collected are only for O_3.

A wrapper code that reads the field study data and calls the standalone dry deposition scheme will be provided as an optional runtime environment. Alternatively, participants may submit documented computer code (Fortran) of their deposition scheme that interfaces with the provided wrapper code. This will allow the box model planning team to run the scheme. Predictions will be compared between schemes and evaluated against available observed ozone deposition velocities.

Perturbation simulations: The second part of this effort will explore the sensitivity of the modeled deposition values to inputs such as land use type, leaf area index, surface wetness, soil moisture, and humidity. Participants are asked to recalculate and report dry deposition under specified conditions provided for each sensitivity test. Optionally, participants may submit their code and the perturbation simulations will be run by the AQMEII4.A3 planning team.

Iterative approach: The analysis is expected to have an iterative aspect because the initial simulations may suggest further sensitivity simulations to better answer the science questions. The computational time required for simulations is expected to be small (see below). Monthly conference calls are planned to help discuss and develop the analysis. Additional simulation suggestions from the participant community are welcomed.

Data site: A dedicated site for the transfer of files for this effort has been set up at the US Environmental Protection Agency. Participants must first register to obtain a username and then will be granted access to the site for downloading input data and uploading output data and code. Please note that use of the ozone flux observational datasets will often require collaboration and co-authorship with the group who performed the measurements. There is a separate data use policy for each site. Instructions for data site access are below.

1. Go to https://waa.epa.gov and click on “Self Register”.
2. You should now see a form for EPA Web Application Access Self Registration. The EPA Contact information is as follows:

   EPA Contact Name: Donna Schwede
   EPA Contact’s Email Address: Schwede.donna@epa.gov
   EPA Contact’s Phone Number: 919-541-3255
3. Complete the entries for your information and select a password.

4. You will also be asked to select the Community or Application for which you are requesting access. Select "**General Web Application Access**" from the list.
5. Check the box to accept the EPA Privacy & Security Notice.
6. Click "Submit Registration".
7. You should receive a confirmation of your registration via email and you will also be sent your username via email.
8. Send your username to Donna Schwede (schwede.donna@epa.gov) so that you can be granted access to the AQMEII 4 site.
9. You will receive an email indicating that you have been granted access to the AQMEII4 site.
10. Once you have been granted access to the AQMEII4 Data Site, please log in at https://goanyd01.epa.gov/webclient/Login.xhtml using your username and password.
11. You should then be able to go to the AQMEII4 main folder. There are subfolders for
    a. Box Model Code
    b. Box Model Results
    c. Flux Datasets
12. You should have access to all 3 folders. Please download and upload data and model code as needed.

Anticipated work required of participants

The planning team will minimize the burden on participants by specifying all simulation conditions in a standard format (e.g. csv or text files). We will also provide a wrapper program (e.g. Fortran or python) to help automate the process of running the dry deposition schemes, including all sensitivity simulations. The participants are responsible for creating the standalone dry deposition code. This may be as simple as extracting the code from the regional model. Since the requested deposition velocities and resistance/conductance components are the same as specified for the AQMEII 4.A1 full grid modeling activity, the coding burden will hopefully be minimal. Since dry deposition algorithms are very fast, this activity has very minimal computational burden, even with several perturbation simulations. Participants are invited to lead and participate in subsequent analyses and author or co-author publications. As with the flux data sets, appropriate co-authorship should be offered to those whose modeling data may be used in a publication.

Information requested from participants

- Deposition velocities and resistance/conductance components for trace gases and aerosols as listed in Table 2. If your dry deposition scheme does not include a listed term, please archive a missing value of -999.99.

- Documentation of dry deposition algorithm, including all equations, input baseline parameter values (e.g. minimum stomatal resistance, chemical diffusivity) and implementation details. Documentation should include relevant references as well as summary of the equations used in the deposition velocity calculation. Examples are shown in Table 3.
- Submission of source code for dry deposition schemes is encouraged to facilitate analyses.

If you are interested in participating in this exercise, please contact Donna Schwede (schwede.donna@epa.gov) or Olivia Clifton (oclifton@ucar.edu).

Planning team

Olivia Clifton, Lisa Emberson, Johannes Flemming, Christopher Holmes, Paul Makar, Sam Silva, and Donna Schwede

Table 1. Measurement variables to be provided.

Parameter	**Time resolution**	**Units**
Air temperature	Hourly (or half-hourly)	ºC
Relative humidity	Hourly (or half-hourly)	Fractional
Ambient pressure	Hourly (or half-hourly)	hPa
Shortwave radiation	Hourly (or half-hourly)	W m^{-2}
Photosynthetically active radiation	Hourly (or half-hourly)	micromoles m^{-2} s^{-1}
Net radiation	Hourly (or half-hourly)	W m^{-2}
Friction velocity	Hourly (or half-hourly)	m s^{-1}
Wind speed	Hourly (or half-hourly)	m s^{-1}
Wind direction	Hourly (or half-hourly)	Degrees North
Sensible heat flux	Hourly (or half-hourly)	W m^{-2}
Carbon dioxide mixing ratio	Hourly (or half-hourly)	ppm
Precipitation	Hourly (or half-hourly)	mm/s
Leaf wetness	Hourly (or half-hourly)	fractional
Snow cover	Hourly (or half-hourly)	fractional
Near-surface soil moisture	Hourly (or half-hourly)	m^3 m^{-3}
Near-surface soil temperature	Hourly (or half-hourly)	ºC
Leaf area index	Hourly (or half-hourly)	m^2 m^{-2}
Canopy height	Hourly (or half-hourly)	m
Vegetation Description	(background information)	Dominant vegetation types observed at the site
Site latitude, longitude, elevation	(background information)	Site location information

Table 2a. Model outputs to be provided for O_3, SO_2, and HNO_3. Terms are defined in the attached document "AQMEII-4_Reported_gas_phase_deposition_terms_guidance_July15_2019.pdf".

Parameter	**Units**
Deposition velocity	cm/s
Aerodynamic Resistance	s/cm
Bulk surface resistance	s/cm
Net stomatal resistance	s/cm
Net mesophyll resistance	s/cm
Net cuticle resistance	s/cm
Effective conductance associated with deposition to plant stomata	s/cm
Effective conductance associated with deposition to plant cuticles	s/cm
Effective conductance associated with deposition to soil and unvegetated surfaces	s/cm
Effective conductance associated with deposition to the lower canopy	s/cm
Quasi-laminar sublayer resistance associated with *stomatal pathway* (= rb if this is pathway-independent for the deposition framework)	s/cm
Quasi-laminar sublayer resistance associated with cuticle pathway (= rb if this is pathway-independent for the deposition framework)	cm/s
Quasi-laminar sublayer resistance associated with soil pathway (= rb if this is pathway-independent for the deposition framework)	cm/s
Quasi-laminar sublayer resistance associated with lower canopy pathway (= rb if this is pathway-independent for the deposition framework)	cm/s
Resistance associated with within-canopy turbulence	cm/s

Table 2b. Model outputs to be provided for a 0.1µm, 1 µm and 10 µm diameter aerosol. For purposes of this exercise we will assume a constant diameter with no additional hygroscopic changes. For each diameter, densities of 1.0 g cm^{-3} and 2.2 g cm^{-3} are to be used.

Parameter	**Units**
Deposition velocity	cm/s
Gravitational settling velocity	cm/s
Aerodynamic resistance	s/cm
Quasi-Laminar Sublayer Resistance	s/cm
Surface Resistance	s/cm

Table 3. Example documentation of model equations for deposition schemes. Definitions for all variables and parameters should be provided. Note that these are examples, and additional modeling details may be provided for the models below at submission.

	Zhang	CMAQ-M3DRY	WESELY
Modeling framework	$V_d(z) = (R_a(z) + R_b + R_c)^{-1}$	$V_d(z) = (R_a(z) + R_b + R_c)^{-1}$	$V_d(z) = (R_a(z) + R_b + R_c)^{-1}$
Aerodynamic resistance (R_a)	For stable conditions, $$R_a = \frac{0.74\, ln(\frac{z}{z_0}) + 4.7\frac{z}{L}}{\kappa u_*}$$ For unstable conditions, $$R_a = \frac{0.74}{\kappa u_*}\left[ln\left(\frac{z}{z_0}\right) - 2\, ln\left(\frac{\sqrt{1-9\frac{z}{L}}+1}{2}\right)\right]$$	$$R_a = \frac{0.95\left[ln(\frac{z}{z_0}) + \psi_h\left(\frac{z}{L}\right) - \psi_h\left(\frac{z_0}{L}\right)\right]}{\kappa u_*}$$ For stable conditions, $$\psi_h = 5\frac{z}{L}$$ For unstable conditions, $$\psi_h = -2\, ln\left(\frac{\sqrt{1-16\frac{z}{L}}+1}{2}\right)$$	For stable conditions, $$R_a = \frac{0.74\, ln(\frac{z}{z_0}) + 4.7\frac{z-z_0}{L}}{\kappa u_*}$$ For unstable conditions, $$R_a = \frac{0.74}{\kappa u_*}\left\{ln\left[\frac{\sqrt{1-9\frac{z}{L}}-1}{\sqrt{1-9\frac{z}{L}}+1}\right] - ln\left[\frac{\sqrt{1-9\frac{z_0}{L}}-1}{\sqrt{1-9\frac{z_0}{L}}+1}\right]\right\}$$
Quasi-laminar sub-layer resistance (R_b)	$R_b = 2(\kappa u_*)^{-1}(D_\theta/D_c)^{2/3}$	$R_b = 2(\kappa u_*)^{-1}(S_c/P_r)^{2/3}$	$R_b = 2(\kappa u_*)^{-1}(S_c/P_r)^{2/3}$
Stomatal resistance (R_s)	$$R_s = \frac{R_s(PAR)}{f_T f_{vpd} f_w}$$ $$\frac{1}{R_s(PAR)} = \frac{LAI_{sun}}{r_s(PAR_{sun})} + \frac{LAI_{shade}}{r_s(PAR_{shade})}$$	$$R_s = \frac{r_{s,min}}{LAI f_{PAR} f_T f_{vpd} f_w}$$	$$R_s = R\left\{1 + \frac{1}{[200(R_G+0.1)]^2}\right\}\frac{400}{T_s(40-T_s)}_{s,min}$$

	$r_s\left(PAR\right)=\frac{r_{s,\min}}{f_{PAR}}$		
Cuticular resistance (R_{cut})	For dry surface, $$R_{cut}=\frac{R_{cutd0}}{e^{0.03RH}LAI^{0.25}u_*}$$ For wet surface, $R_{cut}=\frac{R_{cutw0}}{LAI^{0.5}u_*}$	For dry surfaces and chemical species other than O_3, $$R_{cut,dry}=R_{cut0}*a0/ar$$ For O_3 deposition to dry surfaces, $$R_{cut}=R_{cut,dry}(1-F_{RH})+R_{cut,wet}\times F_{RH}$$ $$F_{RH}=\frac{(RH-70)}{30}$$ For wet surfaces (not frozen), $$R_{cut,wet}=R_{cw0}/H_{eff}$$ For wet surfaces (frozen). $$R_{cut,wet}=R_{snow}$$	Prescribed values for dry and wet surfaces
In-canopy aerodynamic resistance (R_{ac})	$$R_{ac}=\frac{R_{ac0}LAI^{0.25}}{{u_*}^2}$$	$$R_{ac}=14LAI\frac{h_c}{u_*}$$	Prescribed values
Ground resistance (R_g)	Prescribed values for dry and wet surfaces; adjusted if frozen.	For dry surfaces, $$R_g=R_{g0}+a0/ar$$ For wet surfaces (not frozen),	Prescribed values for dry and wet surfaces; adjusted if frozen.

		$$R_g = R_{gwet0}/H_{eff}$$ For wet surfaces (frozen), $$R_g = R_{snow}$$	

Table 4. Site Vegetation and Soil Characteristics for AQMEII-4 Activity 3 Observation Sites

(Based on references found in Clifton et al., 2019, and other sources of information).

Site Name	Latitude	Longitude	Land use/Land cover	Previous literature
Borden Forest	44 °19'N	79 °56'N	The forest is a natural regrowth from farmland abandoned about 100 years ago. The forest consists of 52% red maple (*Acer rubrum L.*), 14% eastern white pine (*Pinus strobes L.),* 8% largetooth aspen (*Populus grandidentata Michx*.), 7% white ash (*Fraxinus americana L*.), 6% American beech (*Fagus grandifolia*), and 13% other species. The canopy height (h) near the flux tower is approximately 22 m with a peak leaf area index (LAI) of ~4.6 m^2 m^{-2} in summer. Soil Information: "Loose, coarse-textured soils, which have been classified as Tioga sand and sandy-loam. The soils are poor and droughty, and have never been suitable for sustained agriculture."	Makar et al., 2017; Wu et al., 2016 ; Bakowsky et al, 2008.
Bugacpuszta	46.69 ºN	19.60 ºE	*semi-natural semi-arid sandy grassland* Horváth et al., 2018: The plant association is semi-arid sandy grassland (*Cynodonti Festucetum pseudovinae*) dominated by *Festuca pseudovina*, *Carex stenophylla*, and *Cynodon dactylon. Mean LAI =0.5. Soil information: "*The region has Chernozem-type sandy soil with a high sand (79%) and low clay (13%) content in the upper 0.1-m soil layer"	Horváth et al., 2018

Harvard Forest	42.53 ºN	72.18 ºW	*temperate deciduous forest* Munger et al., 1996: Predominantly red oak with red maple, scattered stands of hemlock and white pine, and plantations of red pine. LAI for deciduous trees is 3.4. Wu et al; 2015: The forest is 80 years old on average and consists of red maple (*Acer rubrum*) and red oak (*Quercus rubra*) with scattered stands of Eastern hemlock (*Tsuga canadensis*), red pine (*Pinus resinosa*), and white pine (*Pinus strobus*). The canopy height near the observation tower is up to 23m with a peak LAI of 5.0m^2 m^{-2} during summer. Soil information: "Sandy loam tills (coarse-loamy, mixed, mesic or frigid Typic Dystrocherts or Haplorthods), with or without upland landscape features (drumlins and roche moutonnees), while sandy outwash is found in lower slope terraces and deltas. Muck and peat or till or outwash occurs in closed depressions occurs on low-lying landscape positions."	Clifton et al., 2017, 2019; Munger et al., 1996; Wu, Z. Y., et al., 2015 ; Allen et al., 1995
Hyytiala	61.85 ºN	24.28 ºE	*coniferous forest* Zhou et al, 2017: The boreal coniferous forest is relatively homogeneous around the station in all the directions within 200 m, 75% covered by Scots pine (Pinus sylvestris) and the rest covered by Norway Spruces (Picea abies) and	Altimir et al., 2006; Launiainen et al., 2013; Peltoneimi et al, 2015 ; Rannik et al., 2009, 2012; Zhou, P. T., et al., 2017

			deciduous trees (Bäck et al., 2012). The understory vegetation mainly consists of lingonberry (Vaccinium vitis-idaea) and bilberry (Vaccinium myrtillus) with a mean height of 0.2–0.3 m. The forest floor is covered by dense mosses, mostly Dicranum polysetum, Hylocomium splendens and Pleurozium schreberi. Underneath is a 5 cm layer of humus in soil (Kolari et al., 2006; Kulmala et al., 2008). In 2010, the tree height reaches around 18 m. The all-sided leaf area index (LAI) is about 7.5m^2 m^{-2}, including 6.0m^2 m^{-2} overstorey vegetation, 0.5m^2 m^{-2} understory vegetation and 1 m^2 m^{-2} moss layer. Soil information: Forest soil. "The soil of the catchment consists of haplic podzol formed on glacial till, with average organic layer thickness of 5 cm… the effective depth of the soil in terms of soil water dynamics is 413 mm."	
Ispra	45.8126ºN	8.6336ºE	Deciduous forest	
Ramat Hanadiv	32º33'19.87''N	4º56'50.23ºE	*shrub 3.6 km away from eastern Mediterranean seashore* Li et al., 2018: Vegetation surrounding the measurement site is dominated by Eastern Mediterranean shrubbery including: Quercus calliprinos (~25%), Pistacia lentiscus (~20%), the sclerophyll Phillyrea latifolia (broad-leaved phillyrea) (~7.5%) and invasive	Li et al., 2018 ; USDA, 1999.

			species (~10%), Cupressu (5%), Sarcopoterium spinosum (~2%), Rhamnus lycioides (~2%) and Calicotome villosa (~1%). In the west there are a few scattered Pinus halepensis (b5%). The rest of the area is mostly covered by herbaceous vegetation. Typical leaf area index at the site is 1.3 m^2 m^{-2} (measured in fall 2015). Soil information: "The soil type in this area is Xerochrepts, developed from parent rock of hard limestone and dolomite" – Xerochrepts definition (USDA) usually includes something to the effect of "deep, well-drained gravelly soils". Also known as Xeric Inceptisols (xeric - moist cool winters/warm dry summers), or Xerepts, described in the USDA system as "more or less freely drained inceptisols in the xeric moisture regime (USDA, 1999)	

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