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Impacts of Differences in Land Use Characterization and Dry Deposition Schemes on AQMEII4 CMAQ Simulations

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Background

- Since 2009, the Air Quality Modeling Evaluation International Initiative (**AQMEII**) (http://aqmeii.jrc.ec.europa.eu/) has brought together a total of 37 modeling groups from 17 countries in North America and Europe
- AQMEII's goal is to **conduct coordinated research projects and model inter-comparison** exercises aimed at advancing model evaluation practices and informing model development.
- Previous phases have focused on **atmospheric concentrations and meteorological variables**
  - Phase 1 – Initial comparisons and proof of concept
  - Phase 2 – Coupled models; chemistry-meteorology feedbacks
  - Phase 3 – Global to regional modeling; effect of boundary conditions

AQMEII4 Motivation and Objectives

Motivation:

- Deposition remains a crucial process in the species budget of all air quality models, yet has not been systematically evaluated across multiple modeling systems
  - Past studies typically focused on specific modeling systems and deposition totals
- No systematic analysis exists of the individual and combined impacts of different representations of resistances, deposition media, land-use, and meteorological conditions on simulated total deposition

Objectives of AQMEII Phase 4 Grid Model Intercomparison:

- Assess deposition processes in regional-scale models through a diagnostic evaluation and investigate the reasons for differences
- Assess the impact of the diversity of different land types and land type databases on model-estimated deposition
- Determine the range of variability of deposition estimates on a set of common land use (LU) types
- Assess the different methodologies to describe deposition pathways into and onto vegetation
- Assess the range of variability for estimated critical loads and critical load exceedances

Parallel to the grid model intercomparison, AQMEII4 will also conduct a point intercomparison of dry deposition schemes using a collection of ozone flux measurements

AQMEII4 CMAQ Simulations

- **Years:** 2010 and 2016 (this presentation focuses on 2016)
- **Domain:** Contiguous U.S., southern Canada, northern Mexico at 12 km resolution
- **Model Version:** CMAQv5.3.1*
  - CB6r3 chemical mechanism, aero7 aerosol scheme, bi-directional NH_3 flux
  - Dry Deposition: M3DRY and STAGE*
- **Meteorology:**
  - WRFv4.1.1 w/o lightning assimilation, MODIS LU
  - 2016 sensitivity: WRFv4.1.1 w/ NLCD40 LU
    - For MODIS, leaf area index and vegetation fraction were obtained from lookup tables while for NLCD40, these parameters were obtained directly from MODIS satellite products following Ran et al. (2016)
- **Emissions:**
  - Anthropogenic: 2010eo and 2016ff modeling platforms
  - Biogenic: BEIS inline
  - Lightning: GEIA climatology
- **Boundary Conditions:** Copernicus Atmospheric Monitoring Service (CAMS) reanalysis

*See next slide for details

*Use of M3DRY and STAGE for AQMEII4

M3DRY

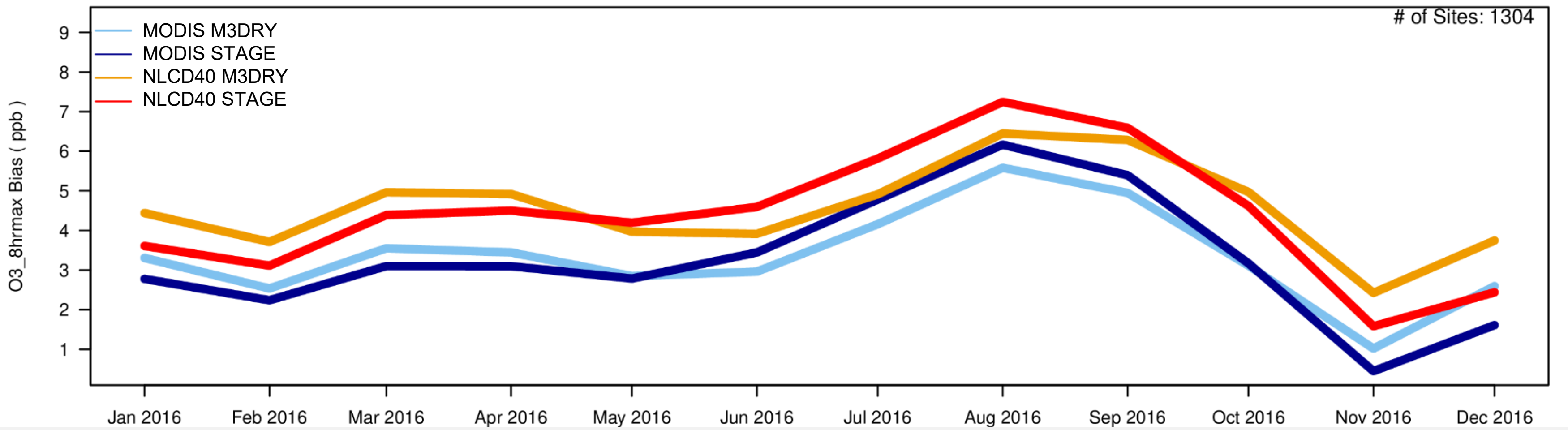
- The AQMEII4 simulations use M3DRY as implemented in the public release of CMAQv5.3.1
- A post-processor has been developed to compute LU-specific dry deposition (DDEP) fluxes and diagnostic variables (deposition velocities - Vd, component resistances, and conductances → slide 11) from standard CMAQ M3DRY output
  - Caveat: M3DRY in CMAQ is designed for maximum consistency with flux calculations in WRF. Specifically, M3DRY computes deposition fluxes at the grid scale and disaggregating these computations to specific land uses in the post-processor involves approximations. The post-processor is designed to maintain grid-scale deposition fluxes but aggregated diagnostic variables may differ from grid-scale values
- Mapping of computed LU-specific deposition fluxes and diagnostic variables from the WRF/CMAQ LU categories to the 16 AQMEII4 LU categories is performed at the post-processing step (→ slide 9)

STAGE

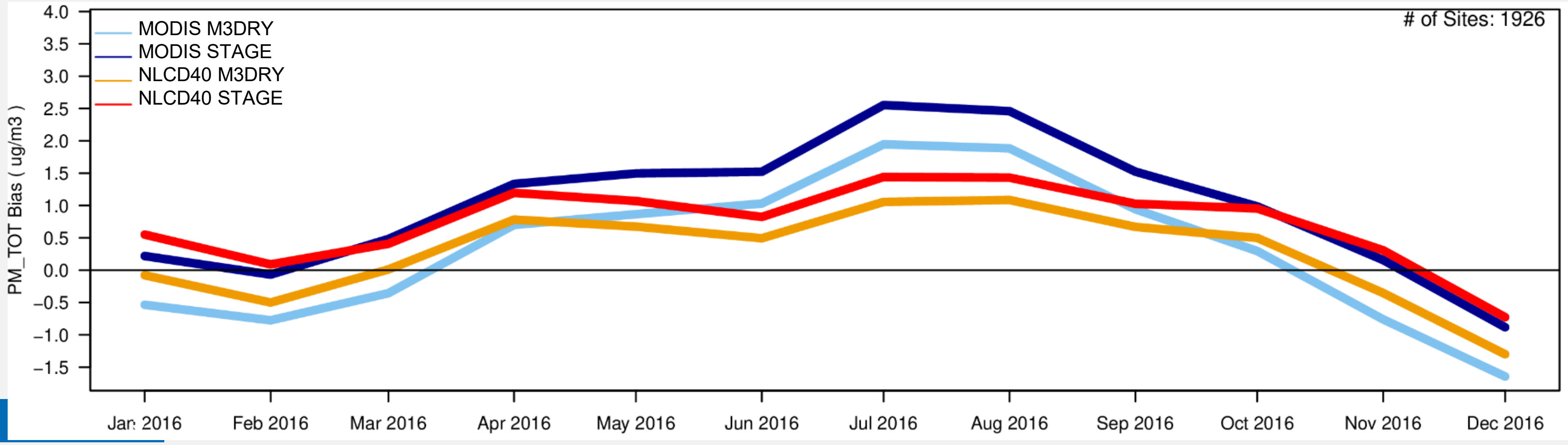
- The AQMEII4 simulations use a customized version of STAGE built on top of the version of STAGE in the public release of CMAQv5.3.1
- The custom version of STAGE calculates and outputs the LU-specific diagnostic variables (Vd, component resistances, and conductances → slide 11) desired in AQMEII4
- The version maps the WRF/CMAQ LU categories and associated deposition-related parameters to the 16 AQMEII4 LU categories (→ slide 9) when performing the dry deposition calculations, i.e. the STAGE dry deposition calculations are being performed directly for the 16 AQMEII4 LU categories

2016 Monthly Mean O_3 and $PM_{2.5}$ Bias Time Series

Monthly Mean Maximum Daily 8-hr Average (MDA8) O_3, All AQS Sites



Monthly Mean 24-hr Average $PM_{2.5}$, All AQS Sites



- The choice of land use and dry deposition schemes can have a noticeable impact on model performance
- The effect of MODIS vs. NLCD40 is comparable to the effect of M3DRY vs. STAGE
- Both simulations using MODIS have lower MDA8 O_3 bias than the simulations using NLCD40

→ Diagnose reasons for differences

→ Focus on O_3 in this presentation

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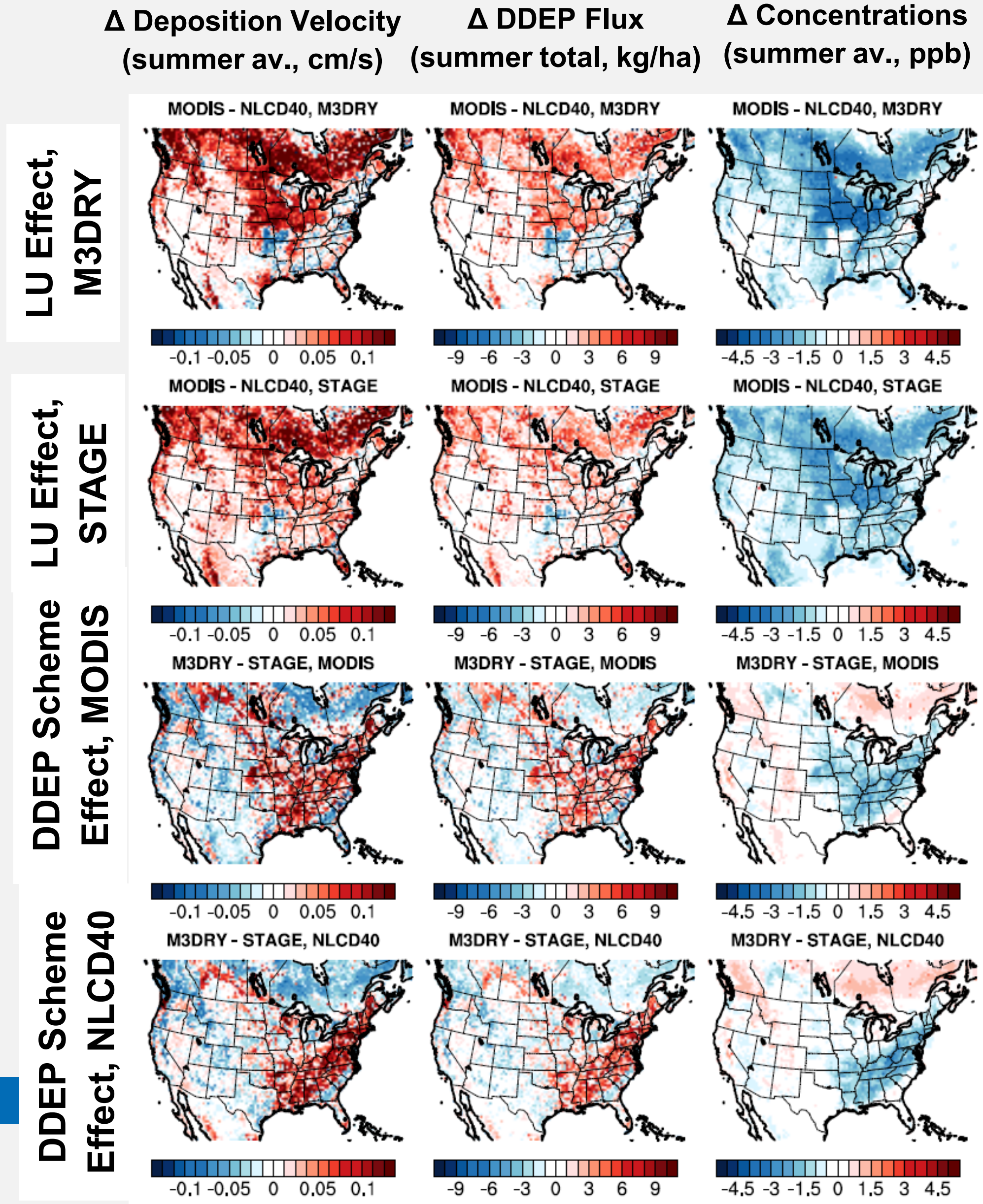
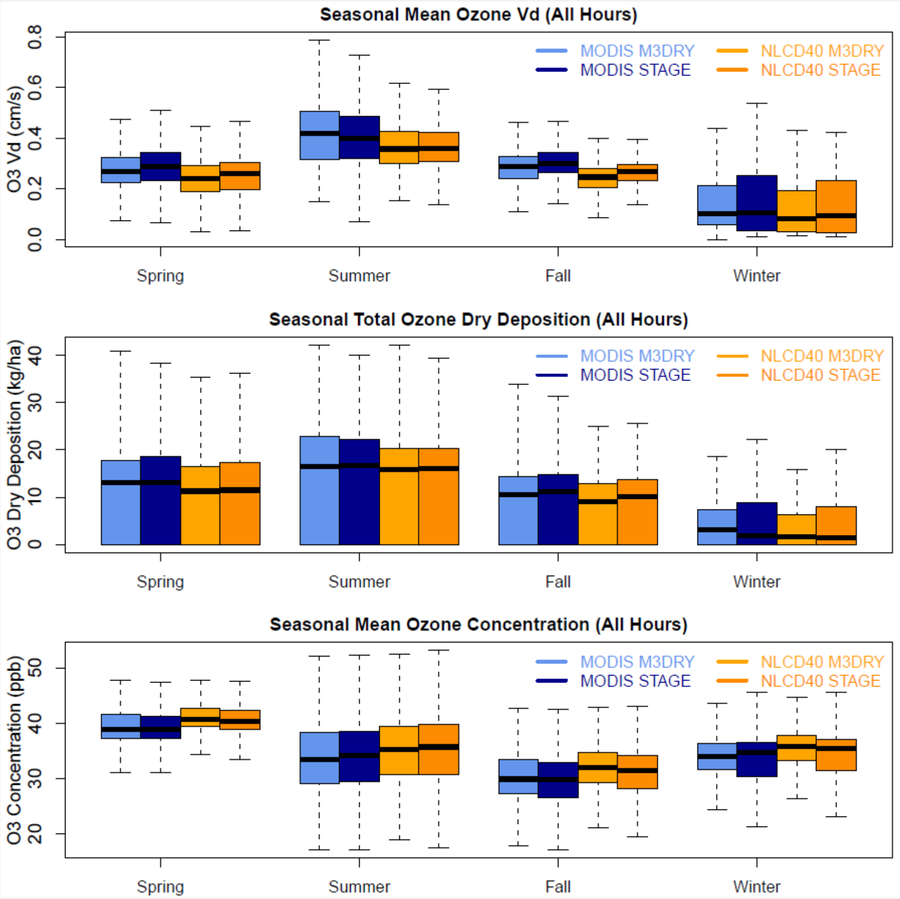
Impacts of LU and DDEP Scheme on O_3 Vd, DDEP Flux, and Concentrations





- The maps and box plots confirm that the patterns and differences in concentrations are linked to patterns and differences in DDEP through patterns and difference in Vd: DDEP = Vd * concentrations
- Both LU differences and DDEP scheme differences affect Vd – perform a diagnostic investigation of the impacts of both

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Effect of MODIS vs. NLCD40 LU Schemes in CMAQ

- LU schemes used in WRF and the dry deposition module of CMAQ affect WRF and CMAQ calculations through the definition of LU types, the spatial distribution of these LU types, and the specification of parameters (surface roughness, u_*, etc.) associated with each LU type
- To enable the comparison of LU specific deposition effects across models, AQMEII4 defined a set of 16 LU types after surveying the LU schemes used by individual groups
- Use the AQMEII4 common LU types to compare the WRF/CMAQ MODIS and NLCD40 simulations for both M3DRY and STAGE

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Mapping of MODIS and NLCD40 LU to AQMEII4

MODIS → AQMEII4

MODIS_Cat	MODIS_Name	AQMEII4_Cat
17	water	AQMEII_01 '
13	Urban and Built-up	AQMEII_02 '
16	Barren or Sparsely Vegetated	AQMEII_03 '
1	Evergreen Needleleaf Forest	AQMEII_04 '
3	Deciduous Needleleaf Forest	AQMEII_05 '
2	Evergreen Broadleaf Forest	AQMEII_06 '
4	Deciduous Broadleaf Forest	AQMEII_07 '
5	Mixed Forest	AQMEII_08 '
6	Closed Shrublands	AQMEII_09 '
7	Open Shrublands	AQMEII_09 '
12	Croplands	'AQMEII_11 '
14	Cropland-Natural Vegetation Mosaic	'AQMEII_11 '
10	Grasslands	'AQMEII_12 '
8	Woody Savanna	'AQMEII_13 '
9	Savanna	'AQMEII_13 '
11	Permanent Wetlands	'AQMEII_14 '
18	Wooded Tundra	'AQMEII_15 '
19	Mixed Tundra	'AQMEII_15 '
20*	Barren Tundra	'AQMEII_15 '
15	Snow and Ice	'AQMEII_16 '

*not present / not used in CONUS12 domain

AQMEII4 LU Categories

AQMEII4_Category	AQMEII4_Description
AQMEII_01	Water
AQMEII_02	Developed / Urban
AQMEII_03	Barren
AQMEII_04	Evergreen needleleaf forest
AQMEII_05	Deciduous needleleaf forest
AQMEII_06	Evergreen broadleaf forest
AQMEII_07	Deciduous broadleaf forest
AQMEII_08	Mixed forest
AQMEII_09	Shrubland
AQMEII_10*	Herbaceous
AQMEII_11	Planted/Cultivated
AQMEII_12	Grassland
AQMEII_13	Savanna
AQMEII_14	Wetlands
AQMEII_15**	Tundra
AQMEII_16	Snow and Ice

*not present in CONUS12 domain with either NLCD40 or MODIS

**not present in CONUS12 domain with NLCD40

NLCD40 → AQMEII4

NLCD40_Cat	NLCD40_Name	AQMEII4_Cat
17	water	AQMEII_01 '
18*	water	AQMEII_01 '
19*	water	AQMEII_01 '
20*	water	AQMEII_01 '
21*	water	AQMEII_01 '
13	Urban and Built-up	AQMEII_02 '
23	Developed open space	AQMEII_02 '
24	Developed Low Intensity	AQMEII_02 '
25	Developed Medium Intensity	AQMEII_02 '
26	Developed High Intensity	AQMEII_02 '
16	Barren or Sparsely Vegetated	AQMEII_03 '
27	Barren Land	AQMEII_03 '
1	Evergreen Needleleaf Forest	AQMEII_04 '
29	Evergreen Forest	AQMEII_04 '
3	Deciduous Needleleaf Forest	AQMEII_05 '
2	Evergreen Broadleaf Forest	AQMEII_06 '
4	Deciduous Broadleaf Forest	AQMEII_07 '
28	Deciduous Forest	AQMEII_07 '
5	Mixed Forest	AQMEII_08 '
30	Mixed Forest	AQMEII_08 '
6	Closed Shrublands	AQMEII_09 '
7	Open Shrublands	AQMEII_09 '
32	Shrub/Scrub	AQMEII_09 '
34*	Sedge/Herbaceous	'AQMEII_10 '
12	Croplands	'AQMEII_11 '
14	Cropland-Natural Vegetation Mosaic	'AQMEII_11 '
37	Pasture/Hay	'AQMEII_11 '
38	Cultivated Crops	'AQMEII_11 '
10	Grasslands	'AQMEII_12 '
33	Grassland/Herbaceous	'AQMEII_12 '
8	Woody Savanna	'AQMEII_13 '
9	Savanna	'AQMEII_13 '
11	Permanent Wetlands	'AQMEII_14 '
39	Woody Wetland	'AQMEII_14 '
40	Emergent Herbaceous Wetland	'AQMEII_14 '
31*	Dwarf Scrub	'AQMEII_15 '
35*	Lichens	'AQMEII_15 '
36*	Moss	'AQMEII_15 '
15	Snow and Ice	'AQMEII_16 '
22*	Perrenial Ice/snow	'AQMEII_16 '

*not present / not used in CONUS12 domain

The same mapping is used in both STAGE (as part of the AQMEII4 CMAQ STAGE configuration) and M3DRY (after post-processor estimation of LU-specific fluxes)

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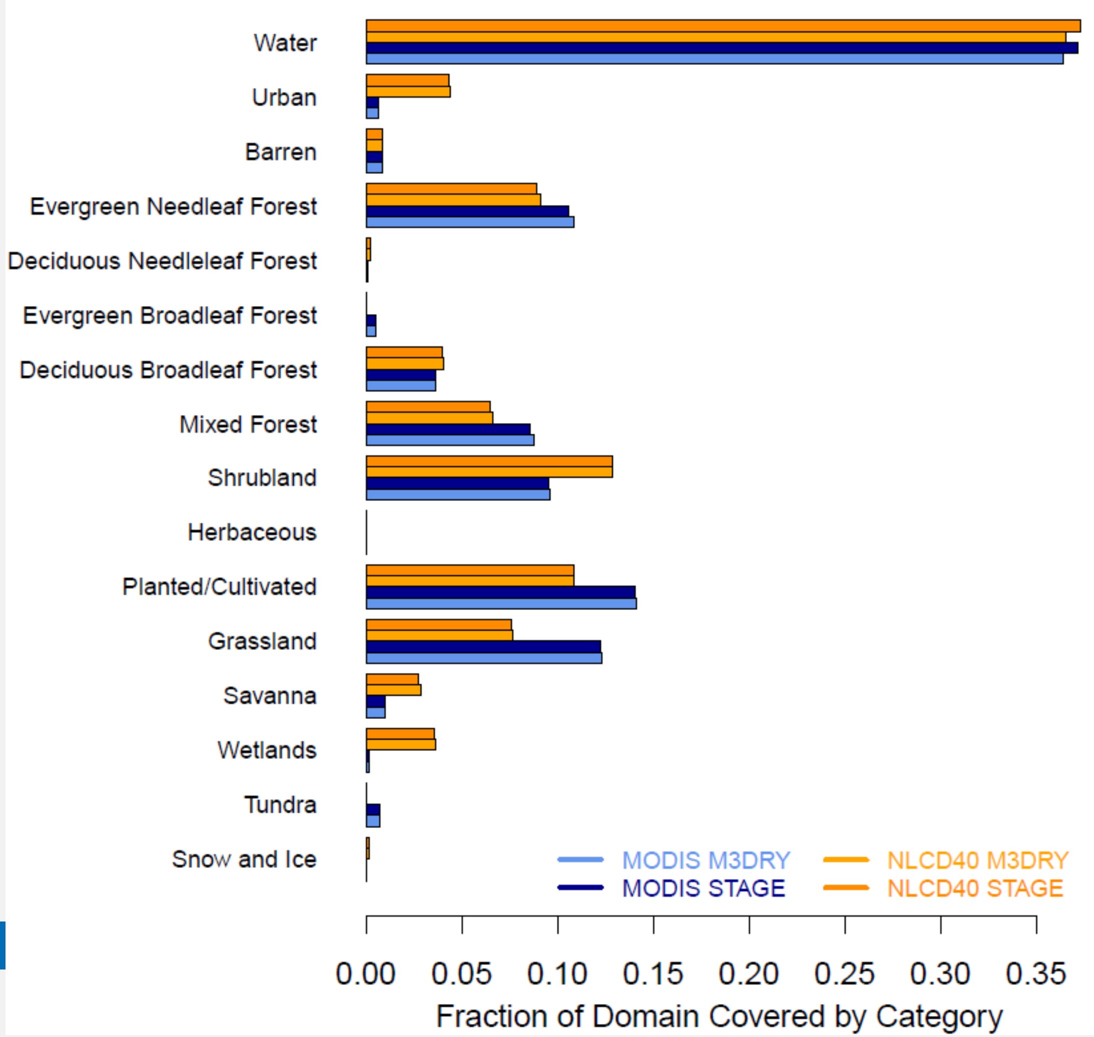
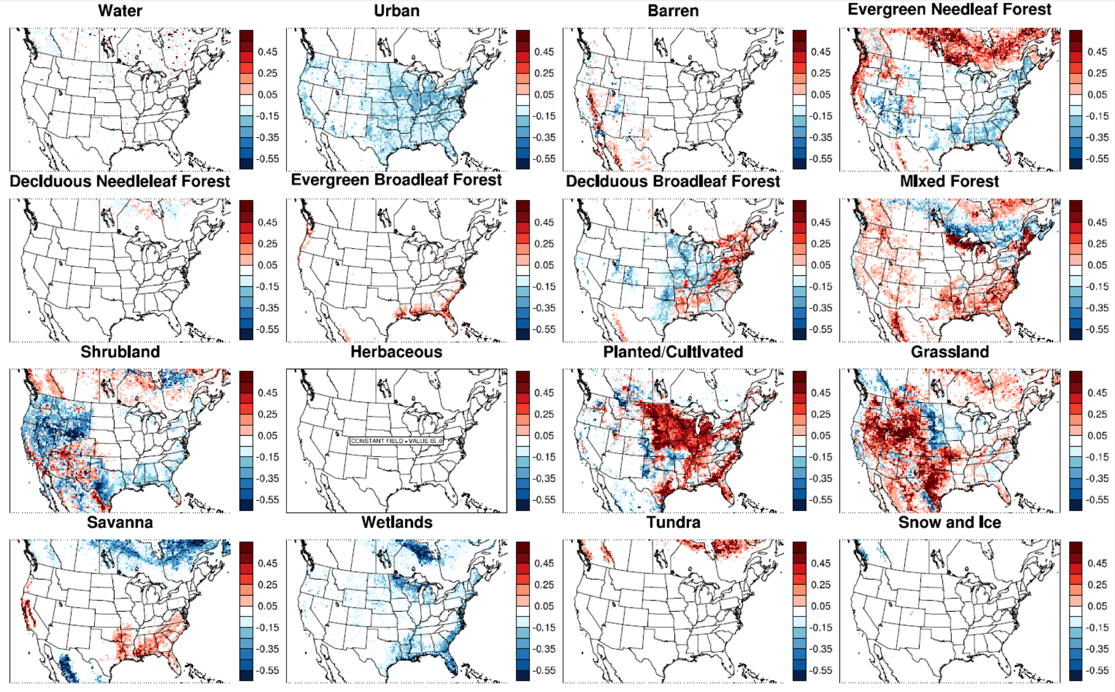
Comparison of MODIS and NLCD40 LU Category Coverages in the 12 km CMAQ Modeling Domain

Fractional Domain-Wide Coverage for Each AQMEII4 LU Category



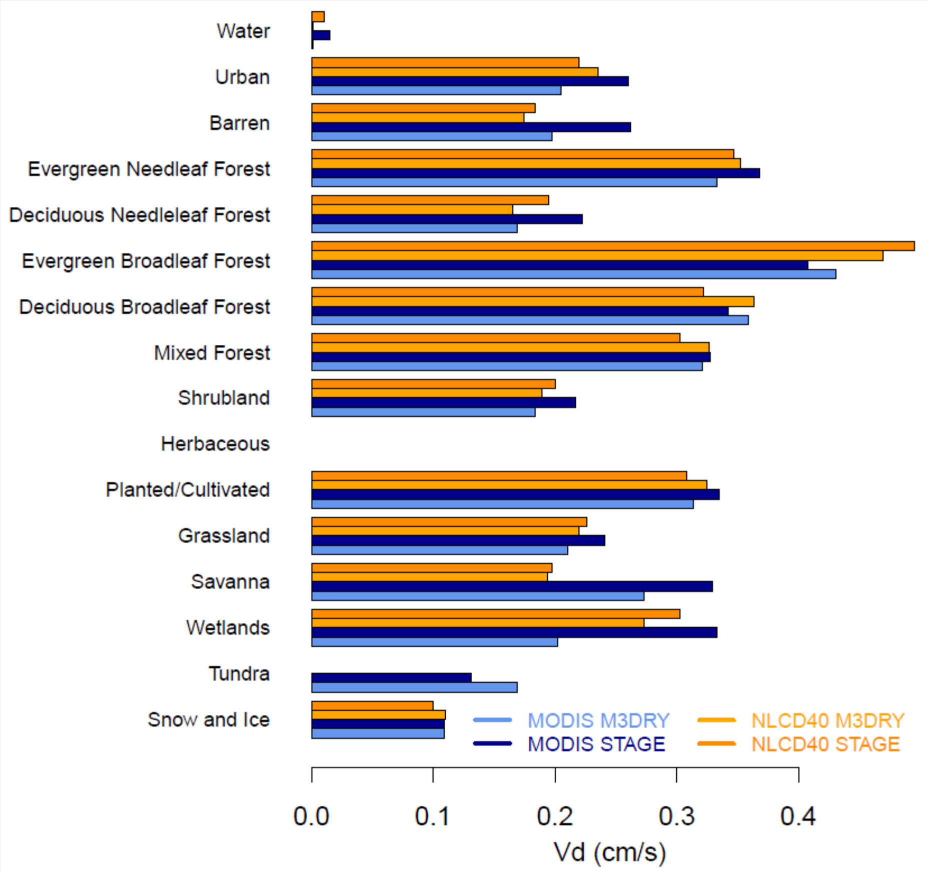
Difference in Fractional LU Coverage MODIS – NLCD40, M3DRY



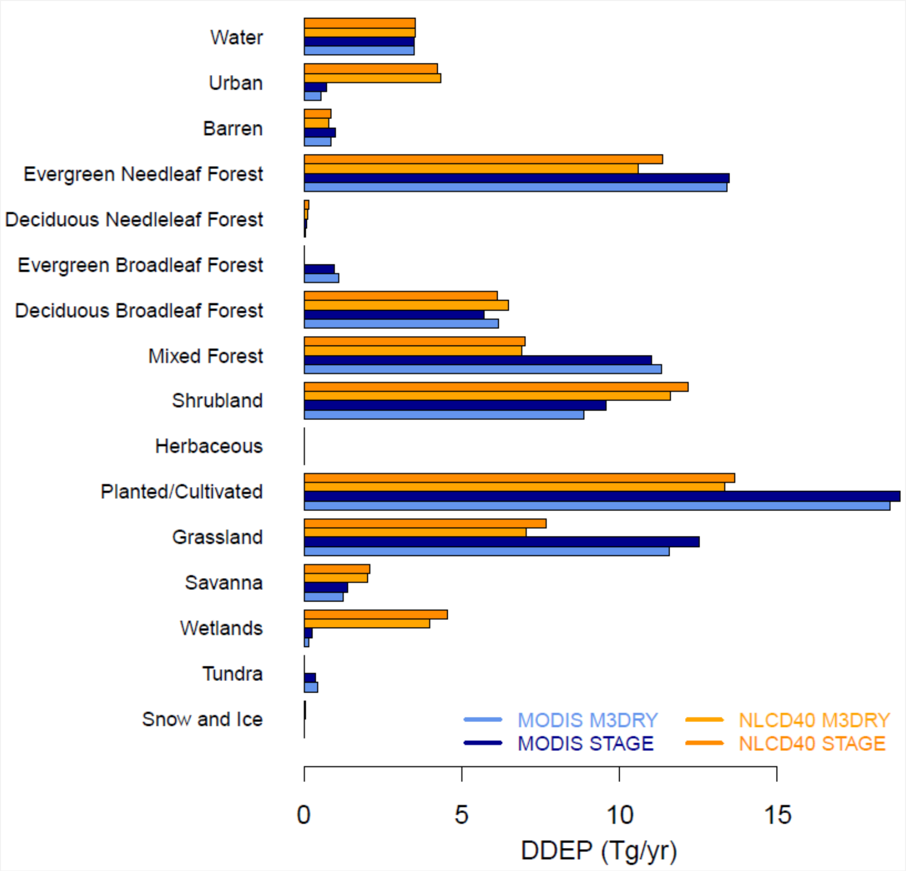
- MODIS has greater fractional coverage for grassland, planted/cultivated, and mixed and evergreen needleleaf forest, and lower coverage for urban and shrubland than NLCD40
- Minor differences in coverage for a given LU scheme between M3DRY and STAGE due to different approaches for representing partial-water grid cells

Comparison of O_3 Vd and DDEP by LU

Annual Mean Vd for Each AQMEII4 LU Category



Annual Mean DDEP for Each AQMEII4 LU Category



Higher fraction of LU categories with higher Vd (e.g. grassland, planted/cultivated, and forests → slide 10) and lower fractions of LU categories with lower Vd (urban, shrubland → slide 10) in the MODIS case result in higher deposition amounts and lower concentrations, both for M3DRY and STAGE

→ the results suggest that the MODIS vs. NLCD40 differences are driven by differences in the fractional coverages of different LU types rather than differences in the specification of LU-specific surface characteristics

Comparing Dry Deposition Across Different Schemes

- While dry deposition schemes in regional-scale models have some resistance terms in common, the details vary considerably across models
- Despite these differences between different resistance formulations, common deposition pathways may be compared using the concept of **effective conductance**
- An **effective conductance** is the contribution of a given depositional pathway to Vd, in the same units as Vd (Clifton et al., 2020):
  - **Four depositional pathways**: **soil**, **lower canopy**, **cuticle** and **stomata**
  - For each pathway, the denominator in the equation to calculate the effective conductance is the inverse of the bulk surface resistance r_c, while the numerator is the inverse of the resistances associated with that pathway in a scheme
  - The formulation of effective conductances thus differs between models, the next slide provides a schematic representation for M3DRY and STAGE
- Once calculated, effective conductances can be used to determine **which deposition pathways** for surface resistance **drive net deposition** and to **characterize** model-to-model, spatial, and temporal **variability in modeled dry deposition**
- This approach is used in AQMEII4 to compare dry deposition across models
- The following slides show the application of this approach to the comparison of CMAQ M3DRY and STAGE

Clifton, O. E., Paulot, F., Fiore, A. M., Horowitz, L. W., Correa, G., Baublitz, C. B., et al. (2020). Influence of dynamic ozone dry deposition on ozone pollution. Journal of Geophysical Research: Atmospheres, 125, e2020JD032398. https://doi.org/10.1029/2020JD032398

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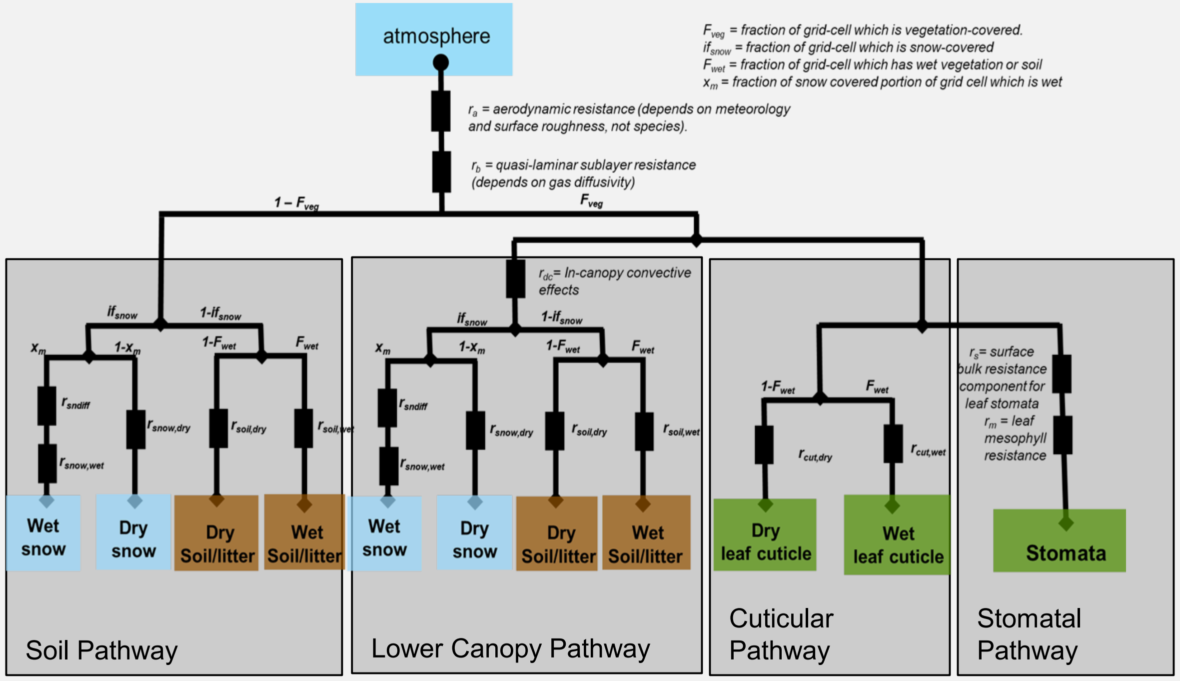
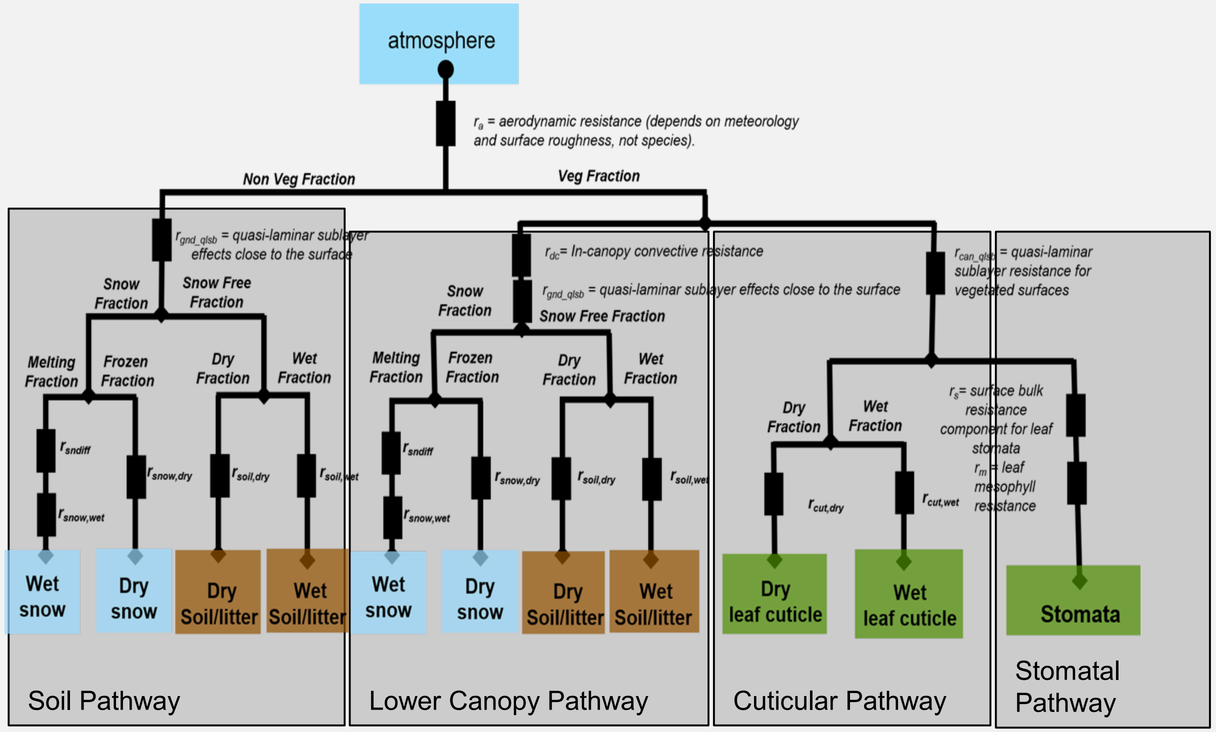
Schematic Representation of M3DRY and STAGE

M3DRY

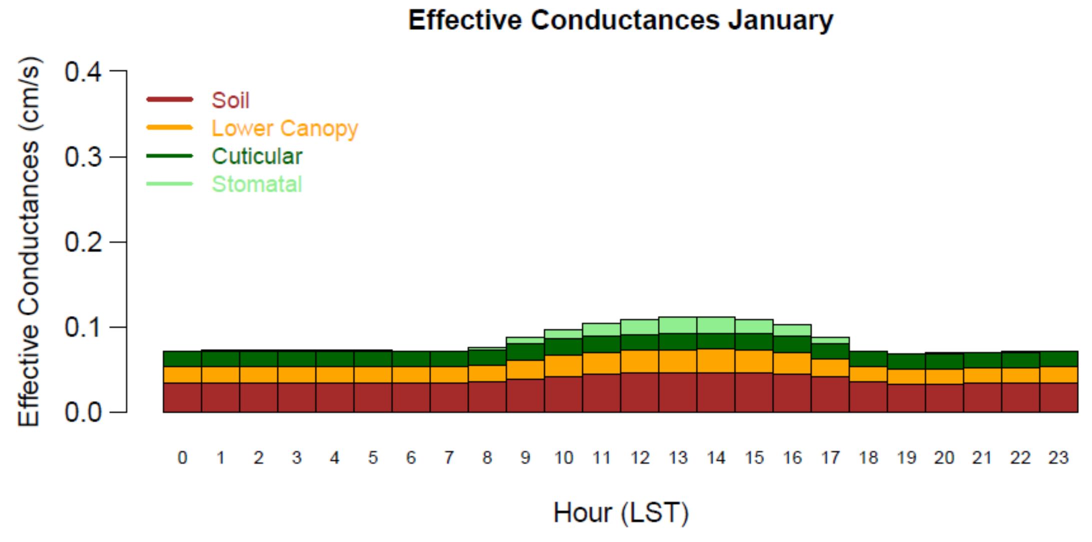


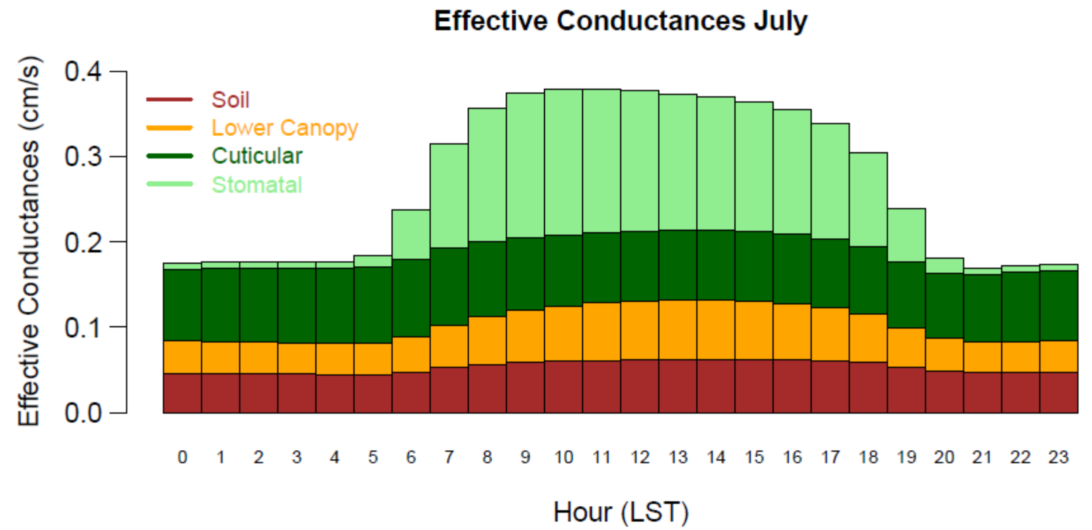
STAGE



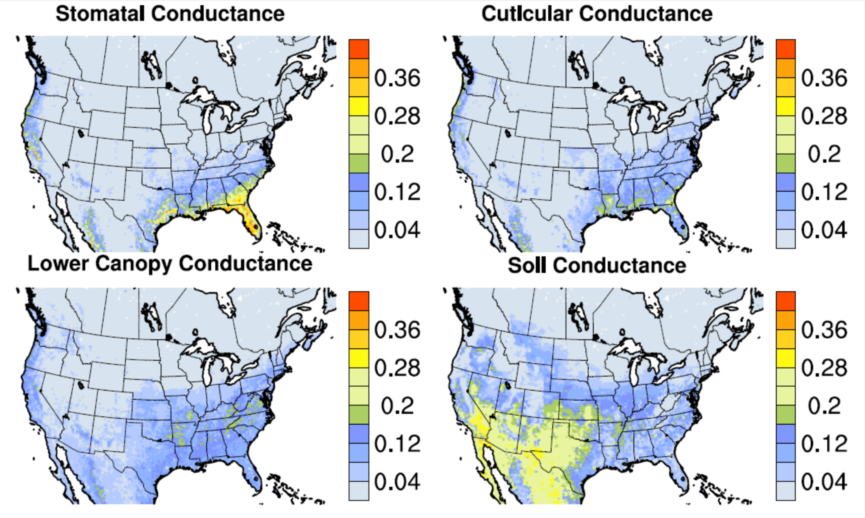
- The main schematic difference is the use of pathway-specific quasi-laminar sublayer resistances in STAGE
- The computation of component resistances (e.g. dry cuticle resistance – $r_{cut,dry}$ or dry soil resistance – $r_{soil,dry}$) differs between both schemes → in addition to computing the four effective conductances, AQMEII4 participants will also provide key resistance value common to most schemes

Spatial and Temporal Variability of Grid-Scale Effective Conductances – Example: MODIS STAGE

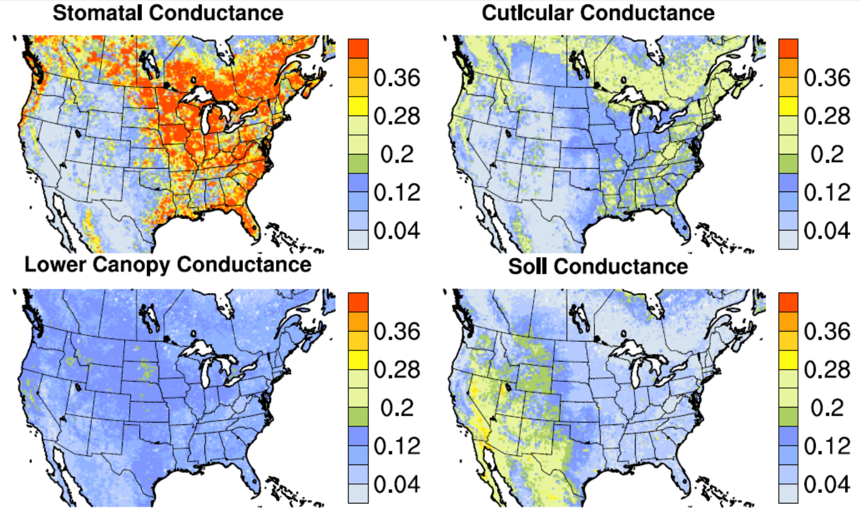




Winter 2 pm (LST) Seasonal Average



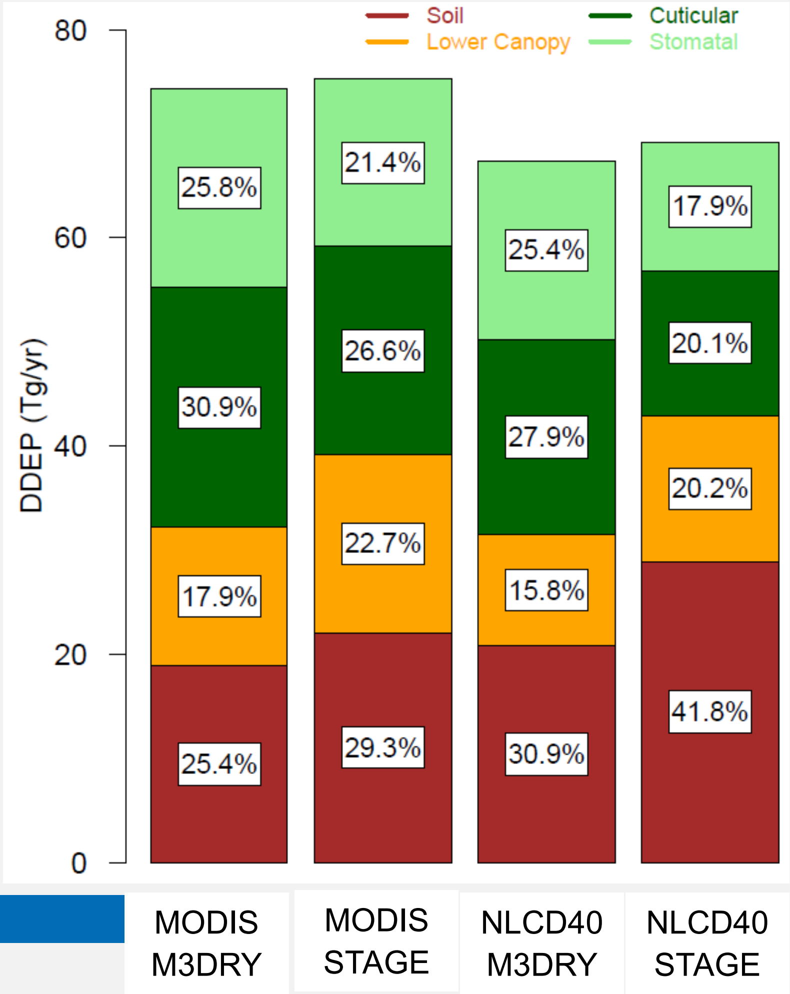
Summer 2 pm (LST) Seasonal Average



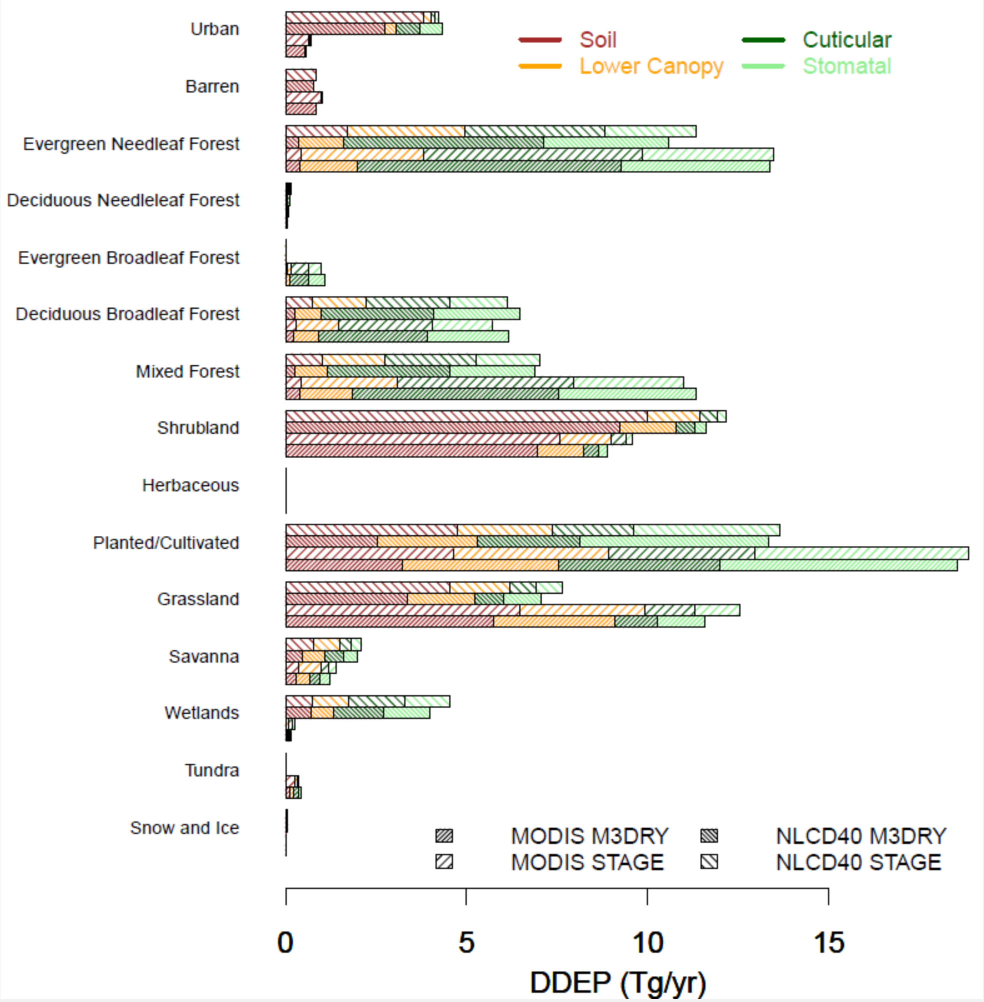
- The magnitudes of the four dry deposition pathways vary diurnally, seasonally, and spatially
- This variation is most pronounced for the stomatal pathway due to its dependence on solar radiation and leaf area
- Similar variability is seen for M3DRY

Annual Total Grid-Scale and LU-Specific O_3 DDEP by Pathway for All Simulations

Annual Domain-Total O_3 DDEP by Pathway (excl. Water Cells)



Annual Domain-Total O_3 DDEP by Pathway and LU (excl. Water)



- Generally greater contribution to DDEP from stomatal and cuticular pathways and lower contribution from lower canopy and soil pathways in M3DRY compared to STAGE
- As expected, the relative importance of pathways varies by LU type due to variations in vegetation coverage
- Comparing pathway and LU-specific Vd and DDEP across models provides diagnostic insights into model behavior
- Such comparisons performed as part of AQMEII4 are also expected to be useful for informing the use of model output for ecosystem impact assessments such as critical load analyses

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Summary

- In the WRF/CMAQ simulations analyzed here, the effects of MODIS vs. NLCD40 LU classification schemes on O_3 are comparable to the effects of different dry deposition modules (M3DRY vs. STAGE)
  - Systematic differences between LU class distributions affect CMAQ dry deposition fluxes
  - The MODIS setup yields consistently lower O_3 than the NLCD40 setup
- Effects of CMAQ dry deposition module (M3DRY vs. STAGE):
  - Generally higher summer O_3 and lower winter O_3 in STAGE than M3DRY
  - Generally greater contribution to DDEP from stomatal and cuticular pathways and lower contribution from lower canopy and soil pathways in M3DRY compared to STAGE
- Comparing pathway and LU-specific Vd and DDEP across models provides diagnostic insights into model behavior
- AQMEII4 will expand this type of analysis across several other air quality models and their deposition schemes