Study of the Impacts of Dry Deposition Schemes in MCIPv2.3 on Deposition Velocity and Concentration of Gaseous Pollutants Using CMAQ

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Dry Deposition

The transport of gaseous and particulate species from the atmosphere onto surfaces in the absence of precipitation.

Factors:

a) Level of atmospheric turbulenceb) Chemical properties of depositing speciesc) Surface characteristics

• $F = -V_d \times C$

Resistance model

 $V_{d} = (R_{a} + R_{b} + R_{c})^{-1}$

R_a - aerodynamic resistance R_b - quasi laminar layer resistance R_c - canopy resistance



Motivations

- Change in V_d can cause O₃ concentration variations upto 20%. (Olerud et al., 1997)
- Dry deposition study important for the Southeast Texas region.
- Two dry deposition schemes in CMAQ v4.4
 a) RADM (*Chang, 1987; Wesely, 1989*)

b) M3DRY (Pleim and Xiu, 2001)

Objectives

- Compare the significance of R_a, R_b, and R_c in the urban and rural regions of Southeast Texas.
- Analyze the differences between dry deposition velocities (V_d) computed by RADM and M3DRY schemes, and its impacts on the gaseous pollutant concentrations.
- Determine a suitable dry deposition scheme for the Southeast Texas region.



Canopy Resistances RADM M3DRY

- 11 landuse categories.
- Soil moisture kept constant for a given season.
- Reactivity compared to that of O₃ (f_{ox}= 0, 0.1, 1.0).
- Resistance calculated based on physical properties or from lookup tables.

Dynamic solar radiation values and soil moisture from MM5PX.

- a) 1-cm surface layer b) 1-m root layer.
- r_{st} parameterized by a) Root zone soil moisture
 b) T_{air} and RH c) PAR
 d) LAI and r_{stmin}.

Domain



- 36km CONUS Domain
- Lambert Conformal Conics
- Domain center: 97 °W, 40 °N
- Vertical Layers: 21



Models and Data

- September 13, 2002 & September 14, 2002
- Emissions inventory: NEI99 Final version 3
- Meteorological model: MM5PX
- Spatial allocator: MIMSβ
- Emissions modeling: SMOKE v2.1
- Meteorology Chemistry Interface Processor: MCIPv2.3
- Chemical transport model: CMAQv4.4
- Chemistry mechanism: saprc99_ae3_aq

Results and Discussion

- Comparison among resistance terms in HGA, BPA, and Rural regions.
- Effect of deposition velocities on pollutant concentrations.
- Flux values of the pollutants.
- Statistical analysis for O₃.

HGA



Conductances from a) M3DRY, and b) RADM for O₃

Canopy Conductance



Canopy Conductance for M3DRY in HGA for O₃

Rural Region



Conductances from a) M3DRY, and b) RADM for O₃

Gaseous Species

Primary importance:

Secondary importance:

- Ozone
- Nitric oxide
- Nitrogen dioxide
- Nitric acid vapor
- Peroxyacetyl nitrate
- Hydrogen peroxide
- Ammonia

- Formaldehyde
- Acetaldehyde
- Dinitrogen pentoxide
- Sulfur dioxide
- Nitrates
- Carbon monoxide
- Nitrous acid
- Sulfate
- Formic acid
- Methyl hydroperoxide
- Peroxyacetic acid
- Methanol
- Generic aldehydes

Ozone Profile in HGA



Ozone in Rural Region



SO₂ Profile in HGA



Daily Average Fluxes

Species	HGA		BPA		RURAL	
	RADM	M3DRY	RADM	M3DRY	RADM	M3DRY
03	1.012	1.565	0.993	1.786	0.773	1.111
NO ₂	0.025	0.142	0.019	0.106	0.005	0.021
SO ₂	0.050	0.141	0.056	0.136	0.022	0.052
H ₂ O ₂	0.027	0.054	0.030	0.053	0.027	0.045
HNO ₃	0.4823	0.4620	0.185	0.180	0.105	0.099

September 13, 2002

Units are in kg km⁻² hr⁻¹

Analysis of O₃ in HGA



Conclusions

- During day-time dry deposition is governed by R_c, and during night-times it is governed by both R_a and R_c for the regions selected.
- V_d differences of 0.4 cm/s (O₃) forces an average concentration difference of 12 ppbv and 10 ppbv for urban and rural areas.
- Daily average dry deposition flux for O₃ from M3DRY is
 1.5 times that of RADM for HGA and Rural.
- M3DRY compares more closely to the observed ozone levels.