CMAQ Sensitivity to Winter-Time Ground Surface Albedo

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1. Introduction

Day-time atmospheric chemistry is driven by sunlight through the photochemical dissociation (photolysis) of molecules into reactive species. O_3 is formed rapidly via dissociation of O_2, but O_3 also plays a complex role in the formation of ammonium nitrate aerosol (NH_4NO_3). The dissociation of O_3 results in an excited oxygen molecule that can combine with H_2O to form the hydroxyl radical (OH). OH can react with NO_2 to form nitric acid (HNO_3) and provide the key ingredient necessary to form particulate NH_4NO_3 via reaction with NH_3.

The probability that a molecule will photochemically dissociate depends on the energy (wave length) of the incident photon. For example, the dissociation of O_3 and NO_2 requires photons in the ultraviolet (UV) range. The number of UV photons impacting a molecule depends on incident (irradiance), reflected, and scattered radiation. Reflected radiation from the ground surface is controlled by ground surface albedo.

The UV ground surface albedo is generally low (< 0.10) for most land use types, but over snow the UV albedo can approach unity (Grenfell et al. 1994). The high UV albedo over snow cover has significant implications for winter-time photochemistry. For example, elevated concentrations of O_3 most commonly occur during the summer, but in the western United States hourly winter-time ozone concentrations in excess of 100 ppb have been observed in western Wyoming and concentrations approaching 60 ppb are common in northern Utah. In these areas, higher UV albedos due to snow cover increase photolysis rates and contribute to elevated gaseous and particulate pollution.

1.1 UV Snow Albedo

Snow cover albedo depends on many factors including age, depth, water content, amount of dirt on the snow surface, and the density of vegetation sticking out of the snow. Tanskanen and Manninen (2007) calculated "effective" UV ground surface albedos over snow covered ground using gridded land use data, gridded snow cover data, and the Total Ozone Mapping Spectrometer (TOMS). They found that certain land use types reduced albedo due to vegetation sticking up through seasonal snow cover. Their findings indicate that average effective UV albedos of snow covered ground can range from 0.83 over bare ground and diminish to 0.72 over grasses, 0.37 over crop lands, and 0.27 over evergreen needleleaf forests.

1.2 CMAQ Photolysis

CMAQ uses a multi step process to calculate photolysis rates. First, JPROC calculates a day specific clear sky photolysis rate look-up table for latitudinal and elevation bands for each photochemical reaction. The calculation utilizes fixed values for spectral ground surface albedo, O_2 and O_3 absorption cross section data, and vertical ozone profiles. Second, CCTM uses the look-up table to interpolate rates to each grid cell location. Finally, CCTM corrects the interpolated photolysis rates to account for attenuation of radiation due to clouds and atmospheric optical depth.

The fixed values of ground surface albedo used in JPROC's photolysis rate calculations are based on work published by Demerjian et al. (1980). This methodology provides unique spectral albedos for 8 wave length bands. The albedos increase from 0.05 for wavelengths less than 400 nm (UV) to 0.15 for wavelengths greater than 660 nm. The fixed spectral albedos work adequately for longer wavelengths, but JPROC's 0.05 albedo for UV wavelengths is not applicable for snow covered ground. The "effective" albedos described by Tanskanen and Manninen (2007) are, at minimum, an order of magnitude larger than what JPROC assumes in the photolysis rate calculation.

2. Methods

Several CMAQ simulations were run to diagnose the sensitivity of model O_3, HNO_3, and NH_4NO_3

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predictions to increased UV albedo. Five sensitivity runs were designed using UV albedos of 0.05, 0.55, 0.65, 0.75, and 0.85. A 4 day simulation was chosen during a January 16-19, 2007 10-day cold pool event that lead to hourly PM2.5 concentrations approaching 100 ug/m3.

JPROC was run using inputs described in the CMAQ user manual including O2 and O_3 absorption cross section data from NASA (DeMore et al. 1994), modified WMO extraterrestrial radiation data, and vertical ozone profiles interpolated from seasonal values. For each JPROC run, the SETALB.F subroutine was hard coded to fix the UV albedo to 0.05, 0.55, 0.65, 0.75, or 0.85.

CMAQ was run for a 4km northern Utah domain that included Salt Lake City and the Wasatch Front. CCTM was configured to use CBV gas phase chemistry and the AERO4 aerosol module. The attenuation of UV radiation by clouds was turned off in CCTM's PHOT.f in order to remove complicating factors related to irradiance fluctuations and reflection from clouds.

3. Results and Discussion

JPROC clear sky NO_2 photolysis rates calculated for a 0.85 UV albedo at 40° N and 2000 meters above MSL increased 85% over the original 0.05 fixed UV albedo (Table 1).

Date	UV Albedo	Rate
July 18	0.05	0.587
January 18	0.05	0.365
January 18	0.55	0.545
January 18	0.65	0.577
January 18	0.75	0.623
January 18	0.85	0.673

Table 1. Photolysis rates calculated by JPROC for several UV albdeo values.

For comparison, a sixth set of photolysis rates were produced using the non-snow covered ground albedo value of 0.05 for July 18. July NO_2 photolysis rates were found to be 15% lower compared to January 18 rates with snow cover and a 0.85 UV albedo.

As expected, CMAQ predictions of O_3, HNO_3, and NO3 concentrations significantly increased during the day-time hours with increased photolysis rates.

Table 2 contains the average and maximum hourly concentration change for January 16-18, 2007 between the hours 1100 MST to 1500 MST for each of the 4 UV albedos tested.

	Average Hourly Concentration Change				
UV Albedo	O3	HNO3	NO3(p)	NH4(p)	NH4NO3(p)
0.55	+17%	+5%	+22%	+15%	+20%
0.65	+21%	+7%	+28%	+19%	+25%
0.75	+26%	+9%	+36%	+24%	+32%
0.85	+30%	+11%	+44%	+30%	+39%
	Maximum Hourly Concentration Change				
UV Albedo	O3	HNO3	NO3(p)	NH4(p)	NH4NO3(p)
0.55	+27%	+14%	+33%	+22%	+30%
0.65	+34%	+17%	+43%	+29%	+38%
0.75	+41%	+21%	+54%	+36%	+48%
0.85	+49%	+26%	+66%	+45%	+59%

Table 2

The concentration increases are large and impact the secondary formation of the NH_4NO_3 aerosol as well as the gaseous molecules. Even at the most conservative albedo of 0.55, maximum O_3 and NH_4NO_3 increases reached +30%.

Figures 1-3 show the entire modeling domain for hour 1400 MST on Janaury 18, 2007. Figures 1a through 1d show the impact of each of the 4 albedo values tested. The area of greatest O_3 increase occurs near urban emissions sources with smaller increases in rural areas.

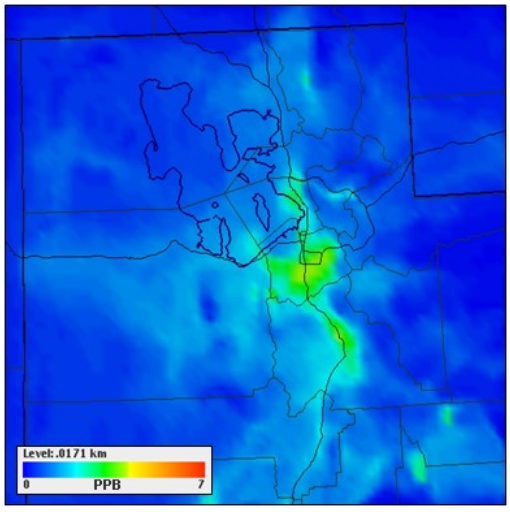

Fig. 1a. O_3 with 0.55 UV albedo.

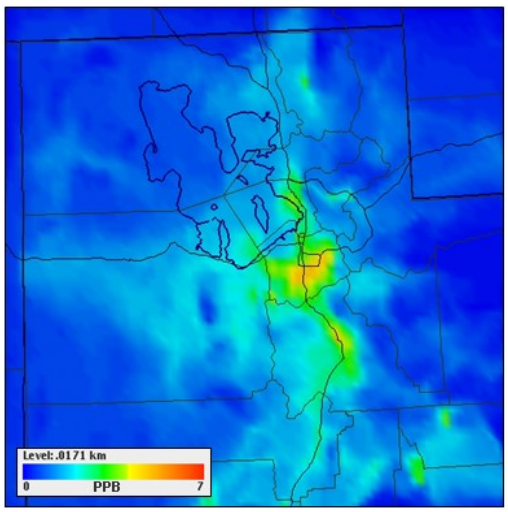

Fig. 1b. O_3 with 0.65 UV albedo.

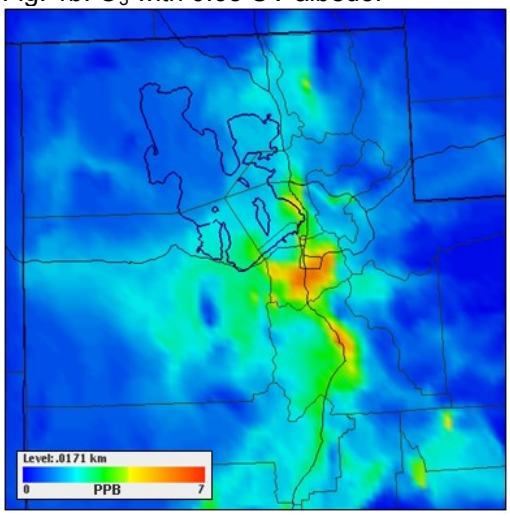

Fig. 1c. O_3 with 0.75 UV albedo.

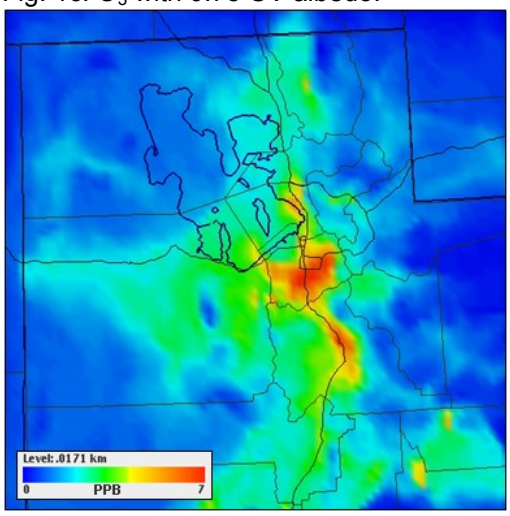

Fig. 1d. O_3 with 0.85 UV albedo.

Figures 2 and 3 show the results from testing an albedo of 0.85. Concentration predictions of HNO_3, the precursor to NH_4NO_3, is shown in Figure 2. It is interesting to note that the grid cells with maximum HNO_3concentration increases do not spatially correspond to the grid cells with maximum NH_4NO_3 concentration increases shown in Figure 3. This may be related to the rate of HNO_3 formation and subsequent reaction with NH_3. The production of HNO_3 from the dissociation of O_3 is not instantaneous and may allow time for advection into neighbor cells before NO_3 is formed.

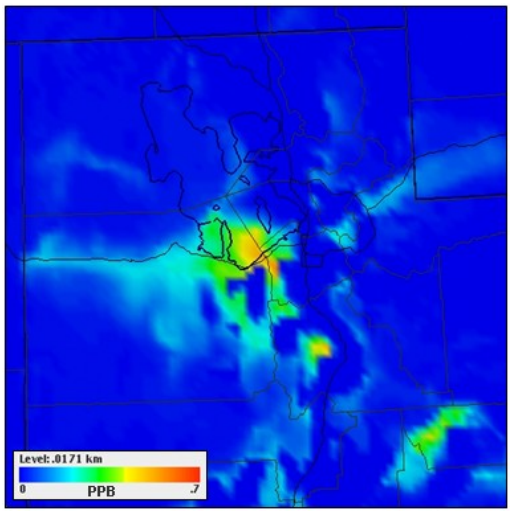

Fig. 2. HNO_3 with 0.85 albedo.

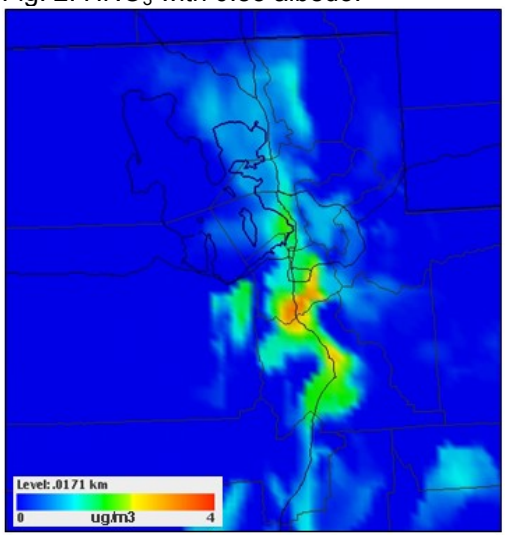

Fig. 3. NH_4NO_3 with 0.85 UV albedo.

4. Conclusion

CMAQ is equipped with a rudimentary fixed value scheme for the calculation of UV photolysis rates. The limitations of the scheme are most pronounced during winter when snow covered ground dramatically increases UV albedo. The winter-time modeling episode presented in this paper demonstrates that the current fixed albedo methodology leads to a significant under prediction of O_3 and secondary $PM_{2.5}$ (in the form of ammonium nitrate). Modeling results suggest that CMAQ needs an improved methodology for adjusting UV ground surface albedo for land use type and snow cover.

5. References

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