Development of CMAQ Boundary Conditions

One of the necessary inputs for performing CMAQ simulations is the boundary condition (BC). The past CMAQ regional photochemical modeling covering episodes relied on the use of 'clean' BCs. Recently, it has been recognized that seasonal and annual simulations, the appropriate BCs can be developed from global models (EPA, 2004). With the development and progress of global chemical transport models such as GEOS-CHEM of Harvard University (http://www-as.harvard.edu/chemistry/trop/geos/index.html) and MOZART of National Center for Atmospheric Research (NCAR) (http://www.acd.ucar.edu/science/gctm/mozart/index.php), it is possible to generate BCs for CMAQ through appropriate interpolation of the global model outputs.

In this note we describe the development of the BCs for the OTC Modeling Committee application of CMAQ at 36 km grid spacing and perform a limited comparison with the BCs reported for Visibility Improvement State and Tribal Association of the Southeast's (VISTA) modeling domain. GEOS-CHEM simulation data for 2002 were obtained through the efforts of the Northeast Consortium of Air Use Management (NESCAUM) in December 2004. The GEOS-CHEM simulation data was at the spatial resolution of 4˚ by 5˚ in the horizontal and 20 layers in the vertical extending from surface to about 100 mb. The model provides information for about 50 chemical gas and particulate matter chemical species. We utilized and modified version of the GEOS-CHEM to CMAQ interface program developed by Prof. Daewon Byun of Huston University so as to match the OTC 36 km modeling domain. To provide an added level of confidence in the development of the BCs, a comparison is performed with the BCs reported for the VISTAs 36 km modeling domain. It should be noted that the two domains differ in their definition with the OTC domain being smaller horizontally and has more layers in the vertical when compared with the VISTA domain.

Spatial patterns of Ozone and SO_4

Figure 1 displays ozone concentrations in layer 1 along the boundaries for OTC and VISTA domains at hour 15 on August 13, 2002. Although the OTC domain is slightly smaller than VISTA domain, both exhibit similar maximum concentration level of about 70 ppb. The OTC domain had slightly higher peak ozone (168 ppb) at the top of the domain along the boundaries than VISTA (see Figure 2), which has a maximum of 139 ppb. This is not unexpected since the top layer of the OTC domain is higher than VISTA domain. Figure 3 shows similar displays for SO_4 at the boundary at the lowest layer of the OTC and VISTA domains.

Averaged Ozone and SO_4 concentrations at the boundaries of the modeling domain

Table 1 lists the averaged ozone concentrations at surface and for the whole boundary layer, (OTC domain with 22 layers, and VISTA domain with 19 layers), at each one of the four boundaries. In both cases the concentrations exhibit similar pattern, with higher concentrations at south and east boundaries and low concentration in the north and west boundaries. Table 2 is similar to Table 1, except it lists SO_4 concentrations. The higher

SO_4 boundary conditions at east direction may be due to the outflow from the US continent.

Averaged Ozone and SO_4 BC vertical profiles from each of the domain

Figure 4 displays the average vertical profile of ozone concentrations at each of four boundaries. As to be expected, GEOS-CHEM yields increasing ozone concentrations with increasing altitude and this is reflected in Figure 4. Figure 5 displays the average vertical profile of SO_4 concentration at each of the four boundaries. The high SO_4 in the East direction may be due to the outflow from the US continent.

References

EPA (2004): Use of GEOS-CHEM for CMAQ Boundary Conditions, http://www.epa.gov/air/interstateairquality/pdfs/GEOSCHEMforCMAQ_Description.pdf

Table 1: The average ozone concentrations at each one of the four boundaries for the OTC and VISTA 36 km domains

Boundary	OTC (22 layer averaged)	VISTA (19 layer averaged)	OTC (surface)	VISTA (surface)
South	43.9 ppb	35.6 ppb	36.8 ppb	31.6 ppb
East	52.2 ppb	46.4 ppb	40.5 ppb	40.7 ppb
North	34.1 ppb	21.9 ppb	13.7 ppb	13.5 ppb
West	40.0 ppb	32.9 ppb	25.8 ppb	24.9 ppb

Table 2: The average SO_4 concentrations at each one of the four boundaries for the OTC and VISTA 36 km domains

Boundary	OTC (22 layer averaged)	VISTA (19 layer averaged)	OTC (surface)	VISTA (surface)
South	0.54	0.51	0.70	0.56
East	1.50	1.67	2.04	1.88
North	0.45	0.54	0.63	0.64
West	0.42	0.47	0.53	0.53

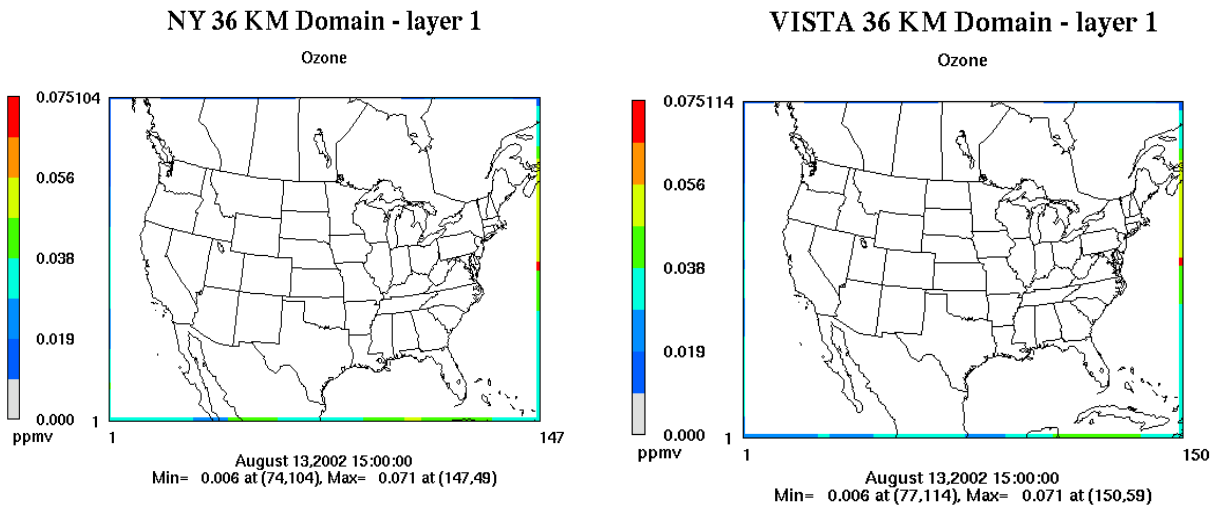

Figure 1: The lowest layer of ozone BC for OTC and VISTA 36 Km domain

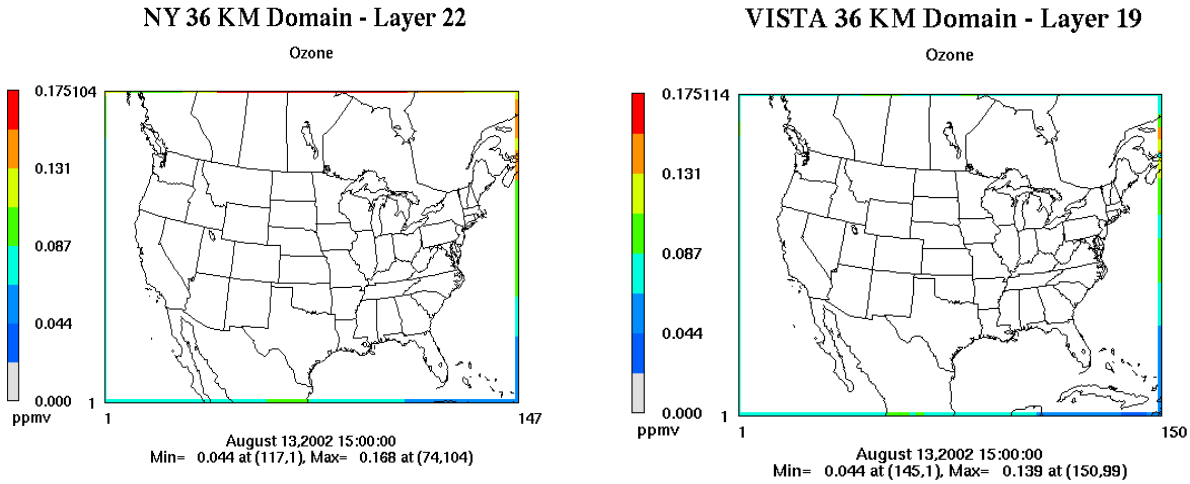

Figure 2: The top layer ozone BC for OTC and VISTA 36 Km domain

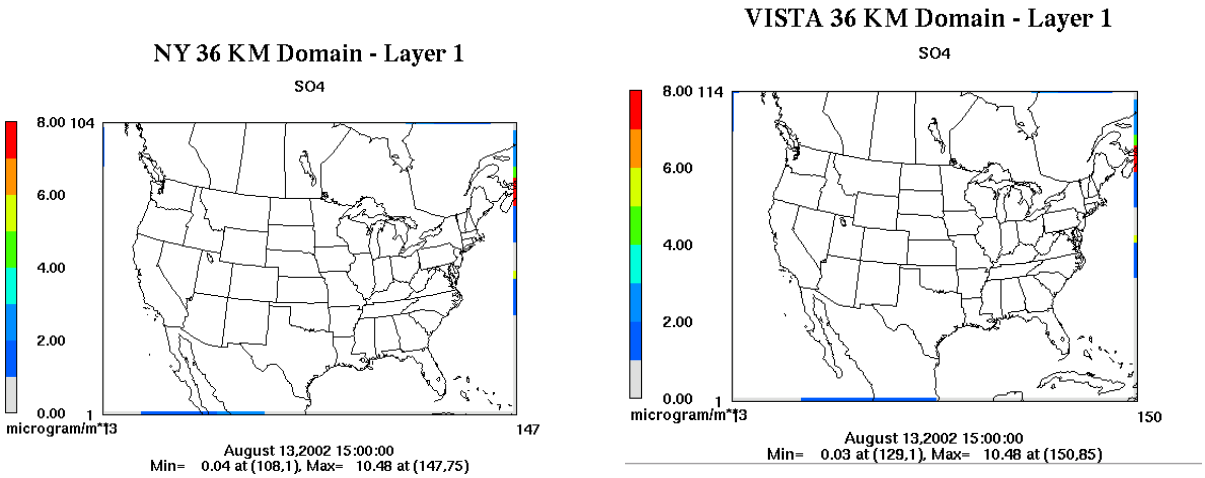

Figure 3: The lowest layer SO4 BC for OTC and VISTA 36 Km domain

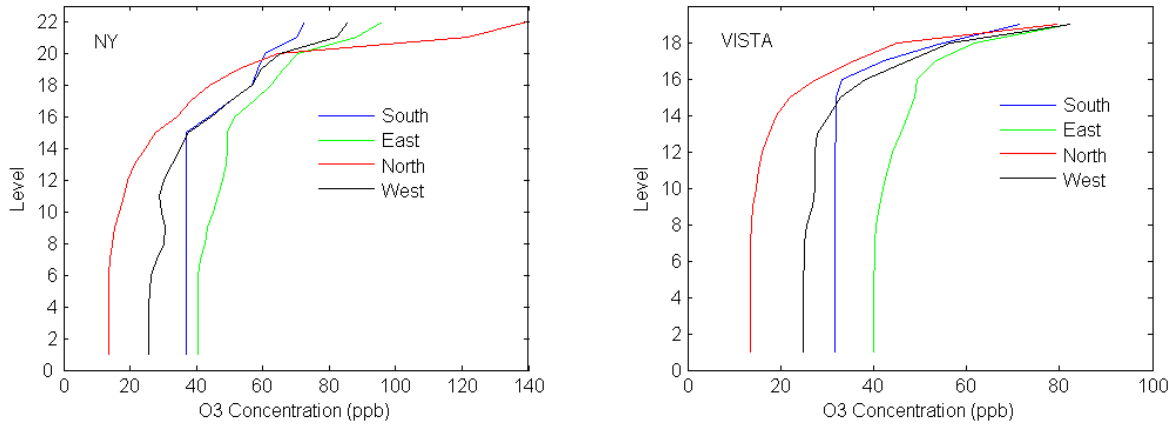

Figure 4: Averaged vertical profiles from each direction of ozone BC

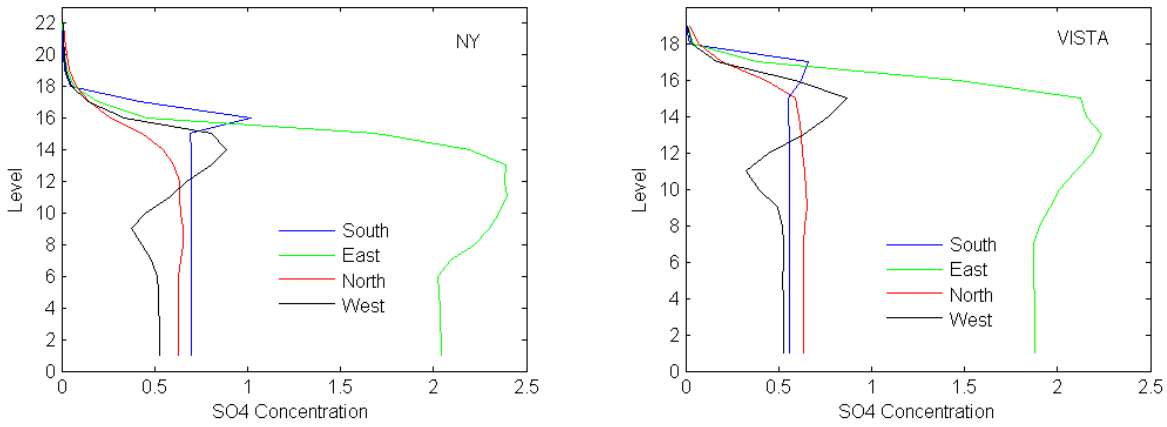

Figure 5: Averaged vertical profiles from each direction of SO4 BC