SENSITIVITY OF AIR QUALITY MODEL PREDICTIONS TO VARIOUS PARAMETERIZATIONS OF VERTICAL EDDY DIFFUSIVITY

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1.INTRODUCTION

This paper investigates the effect of predicted different vertical diffusivity from 3 commonly used PBL schemes on chemical components in the troposphere of East Asia. The 3 schemes are Gayno-Seaman (Shafran et al.,1998), Medium-Range Forecasts (Hong and Pan, 1996), Byun and Dennis (1995)(approach in MCIP/CMAQ), namely GSE, MRF and B&D hereinafter and were incorporated into a regional air quality model (RAQM) to represent vertical mixing process. RAQM is a three-dimensional Eulerian model, which is built on a spherical and terrain-following coordinate system. It represents a series of major processes of chemical components in the troposphere, such as advection, diffusion, dry deposition, cloud and scavenging, gas and aqueous chemistry etc and has been applied to study a number of environmental problems regarding ozone, acid deposition and soil dust transport (Han et al.,2004; Han et al.,2007).

The study domain covers most of East Asia (100ºE-145ºE, 20º-50ºN), with a horizontal grid resolution of 0.5º, and 12 layers extending vertically from surface to 10 km. About 6 layers lie in the planetary boundary layer (PBL). Anthropogenic and biomass emissions are from Streets et al (2003), which is monthly based and on a horizontal grid of 0.5º×0.5º. March 2001 was selected as study period due to the occurrence of significant vertical mixing and availability of high quality observation of TRACE-P aircraft experiment and ground-level observation from Japan site. 3 days prior to March 2001 were taken as spin-up period. Boundary conditions were derived from a global model Mozart II, which provides monthly mean concentrations of several key species including O_3. Model results were evaluated by comparison against the above observations to find out the relative skill of the 3 schemes. Model results using the 3 schemes were also intercompared in terms of vertical diffusivity coefficients and species concentrations to help understand the similarity and discrepancy among them.

TRACE-P aircraft observation comprises a number of important gases and aerosols, with sampling frequency from several seconds to minutes. This study chooses 5 flights which encounter prevailing continental outflow at wide altitudes. For comparison, model results were extracted every 5 minutes and interpolated trilinearly to flight tracks. Statistics measures of correlation coefficient(R), mean bias error

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(MBE), root mean square error (RMSE), normalized mean bias (NMB) and normalized mean error (NME) are calculated for pairs of data to help evaluate model performance.

2. RESULTS

2.1 Statistical analysis

Table 1 shows the statistics for the predicted near surface hourly species concentrations with the 3 schemes at Hedo site of Japan. It is interesting to find that the 3 schemes consistently produce similar correlations for SO_2 (0.59~0.61) and O_3 (0.63~0.65), but more varied correlation for NO_x (0.14~0.25). MRF appears to predict lower SO_2 concentration (with MBE of -0.18 and NMB of -0.26), whereas B&D predicts higher NO_x concentration (MBE 0.53, NMB 0.86). The 3 schemes are very consistent to predict O_3 magnitude, with NMB being 0.27~0.28.

Table 1 Statistics for the predicted hourly species concentrations (ppbv) with the 3 schemes at Hedo site

Scheme	Species	R	MBE	RMSE	NMB	NME
B&D	SO_2	0.61	-0.07	0.55	-0.12	0.68
	NO_x	0.25	0.53	0.75	0.86	0.94
	O_3	0.65	12.35	15.0	0.28	0.30
MRF	SO_2	0.59	-0.18	0.60	-0.26	0.63
	NO_x	0.19	0.46	0.73	0.67	0.79
	O_3	0.64	11.98	14.75	0.27	0.29
GSE	SO_2	0.59	-0.07	0.57	-0.12	0.68
	NO_x	0.14	0.39	0.74	0.52	0.74
	O_3	0.63	12.36	15.1	0.28	0.30

Table 2 shows the statistics for model results in the region of < 2 km by comparison with the TRACE-P aircraft observational data. It is noted that all schemes show a similar skill for SO_2, with R ranging 0.65~0.67, and NMB being 0.14~0.18, but yield relatively large difference in NO_x concentration, with R in a range of 0.29~0.36 and NMB being -0.26~0.04. The consistency for O_3 among the 3 schemes appears to lie between that for SO_2 and NO_x. For <2km region, there is a tendency to overpredict SO_2 and underpredict O_3 concentrations for all schemes, but for NO_x, GSE scheme shows a little overprediction, in contrast to others.

Correspondingly, Table 3 shows the statistics for the region of 2~5 km. The difference in correlation among schemes increases for NO_x, whereas for SO_2 and O_3, the consistency among schemes is similar to that in Table 2. The model skill apparently degrades in the region of 2-5 km compared with that in <2 km region. The significant overprediction for SO_2 is due to the inappropriate treatment of volcano emissions. The predicted higher O_3 concentration is associated with the prescribed O_3 boundary conditions. For NO_x, all schemes show an opposite aspect to that in the < 2km region, with GSE showing underprediction and other 2 schemes exhibiting overprediction.

Table 2 Statistics for the predicted species concentrations with the 3 schemes at altitudes <2 km in the TRACE-P region (ppbv for O_3, pptv for others)

Scheme	Species	R	MBE	RMSE	NMB	NME
B&D	SO_2	0.67	231.6	2526.6	0.15	0.90
	NO_x	0.29	-132.8	690.5	-0.26	0.79
	O_3	0.65	-8.01	15.91	-0.16	0.25
MRF	SO_2	0.65	265.1	2572.6	0.18	0.92
	NO_x	0.30	-81.4	676.3	-0.16	0.81
	O_3	0.62	-8.68	16.80	-0.17	0.26
GSE	SO_2	0.66	217.2	2540.5	0.14	0.88
	NO_x	0.36	21.5	719.8	0.04	0.84
	O_3	0.61	-7.61	16.68	-0.15	0.25

Table 3. Same as Table 2 but for 2-5 km region

Scheme	Species	R	MBE	RMSE	NMB	NME
B&D	SO_2	0.16	491.4	820.4	3.87	4.27
	NO_x	0.21	34.2	234.7	0.32	1.33
	O_3	0.44	13.5	21.5	0.26	0.32
MRF	SO_2	0.18	491.6	798.7	3.88	4.25
	NO_x	0.02	6.1	245.8	0.06	1.22
	O_3	0.43	14.1	22.1	0.27	0.33
GSE	SO_2	0.11	364.8	708.6	2.88	3.48
	NO_x	0.01	-20.6	250.2	-0.2	1.13
	O_3	0.44	13.3	21.3	0.25	0.32

2.2 Spatial distribution

Figure 1 shows the monthly averaged near surface Kz (150m) at 14:00 LST. It is found that MRF scheme produces the largest Kz in the entire domain among all, followed by B&D scheme, and GSE produces the smallest Kz. It appears that the small Kz of GSE near surface inhibit ventilation of SO_2 emission (Figure 2), leading to apparently higher SO_2 concentration than that from the other 2 schemes. The difference in SO_2 concentration between B&D and MRF looks small, although the difference in Kz is apparent between them. Figure 3 shows the monthly mean near surface O_3 concentration predicted with the 3 schemes. The distinctly higher O_3 concentrations in the western parts of domain are due to the influence of constant boundary conditions from the global model. B&D and MRF produce quite similar pattern, with main differences in the southwestern areas of the domain. GSE yields apparently lower O_3 concentration in northeast China and over Tibet than others. However, the 3 schemes appear to be more consistent in the western Pacific Ocean (TRACE-P region). Further analysis of vertical structure of eddy coefficients and associated distribution of species concentrations are undergoing.

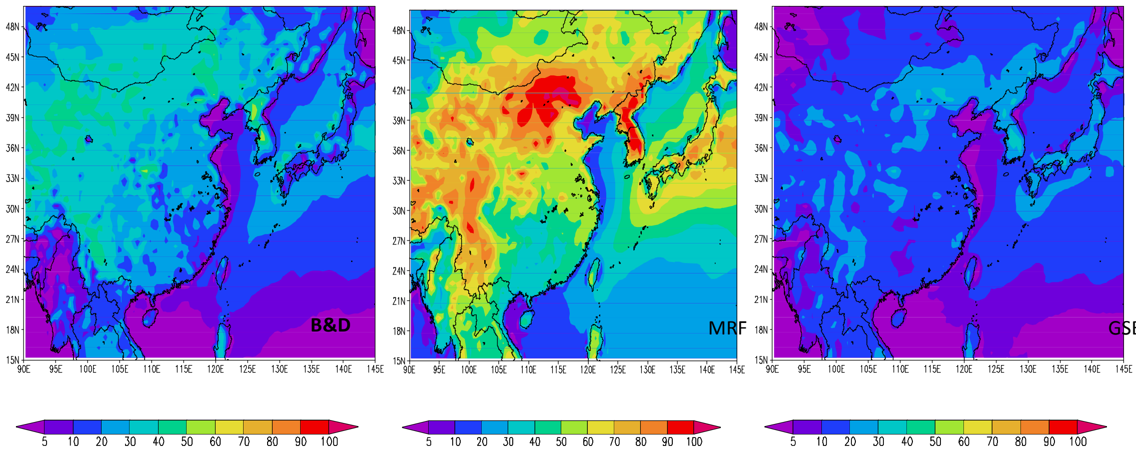

Figure 1 Monthly mean near surface vertical eddy coefficients (150m) at 14:00 LST for the 3 PBL schemes (m^2s^{-1})

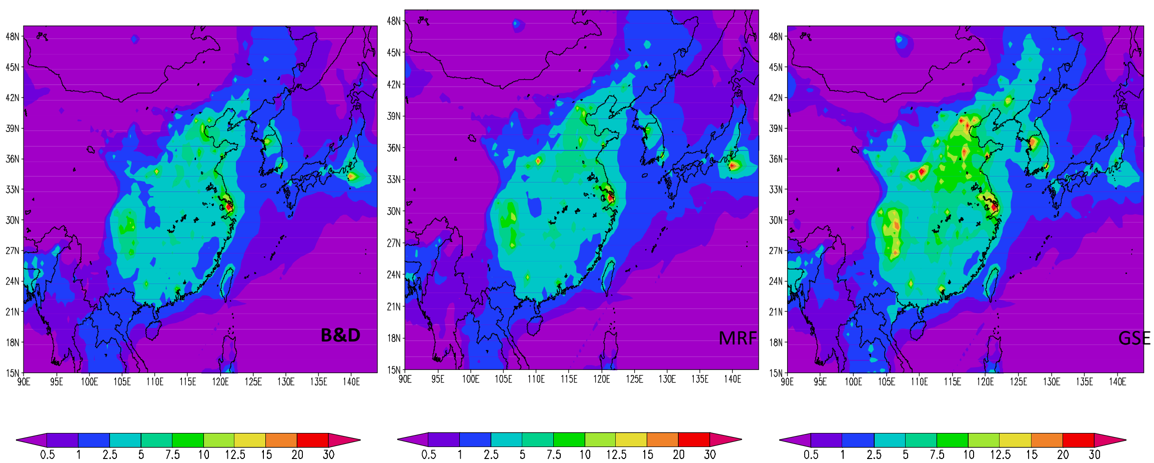

Figure 2 Same as Figure 1 but for SO_2 (ppbv)

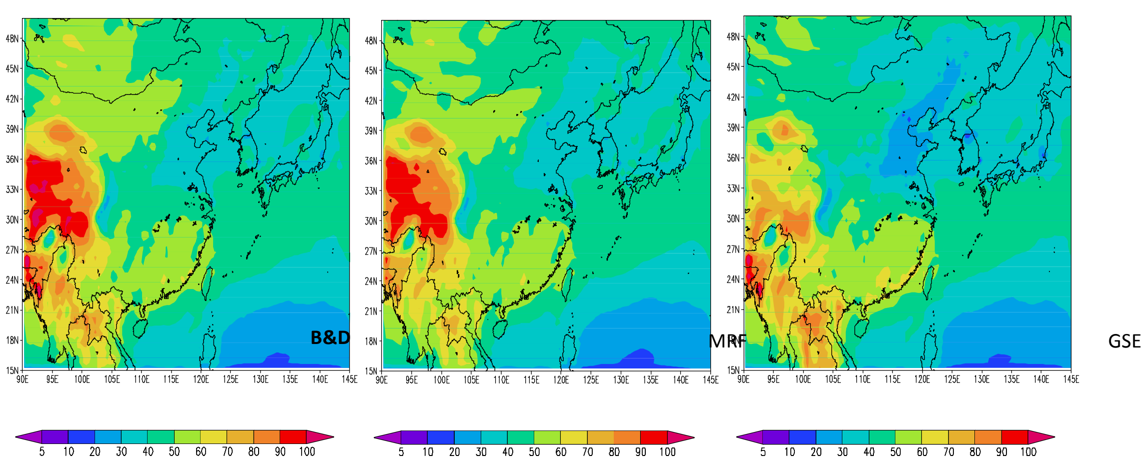

Figure 3 Same as Figure 1 but for O_3 (ppbv)

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