COMPARISON OF CMAQ AND SAQM USING PROCESS ANALYSIS FOR HONG KONG OZONE EPISODES

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1. INTRODUCTION

Rapid development in Hong Kong and neighboring Pearl River Delta (PRD) region of China induces air pollution problems in both places. In 2003 alone, 18 of 31 days of air pollution episodes (Air Pollution Indices that exceed 100) in Hong Kong are due to ozone (Huang 2005). To understand how the high ozone concentration comes about in Hong Kong, numerical models are devised to look at possible individual processes, from mechanics to chemical, and so on. Currently, the Hong Kong Environmental Protection Department (HKEPD) uses PATH modeling system (Pollutants in the Atmosphere and Their Transport in Hong Kong), which consists of meteorological model MM5 and air quality model SAQM. As an alternative to SAQM, CMAQ can serve for comparison in terms of ozone prediction and its associated process analysis. Thus the objective of this study is to examine whether the two models differ qualitatively or the difference is of secondary importance. To facilitate the comparison, identical emission database, identical source of meteorological fields, and identical initial/boundary conditions are input to each of the models. Section 2 provides the model configuration details. Section 3 displays simulation results, which will be summarized and concluded in Section 4.

2. MODEL CONFIGURATIONS

The MM5 fields used consist of four dimensional data assimilaton (FDDA) nudged observations from the Hong Kong Observatory (HKO). The landuse data as an input to the MM5 simulation is also updated by the Hong Kong Lands Department (HKLD) for HK and PRD region in place of the default USGS landuse types. The emission inventories are generated by HKEPD with EMS-95 based on the emission datasets as of 2001. Both MM5 and air quality models (SAQM and CMAQ) are run with a

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configuration of four nested domains (Fig. 1). Horizontal resolutions from the outermost domain to the innermost one are 40.5, 13.5, 4.5, and 1.5 km, respectively. The numbers of grid cells for MM5 nested domains, columns-by-rows, are 115 x 75, 85 x 73, 61 x 55, and 61 x55, while those for PATH and CMAQ nested domains are 49 x 49. In vertical direction, MM5 has 26 unequal sigma layers with 100 hPa at the model top, while SAQM and CMAQ have 15 sigma layers with the lowest 10 coincided with those of MM5.

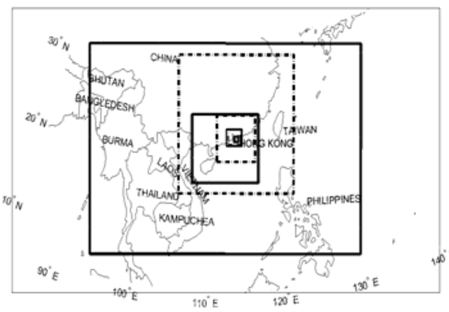

Fig. 1. Settings of four nested domains in MM5 and in SAQM and CMAQ; resolutions from the outmost to the innermost domains are 40.5, 13.5, 4.5, 1.5 km, respectively.

Both air quality models use CB-IV chemical mechanism, but versions are different. SAQM uses the one since its development, while CMAQ uses the one as of default CMAQv4.4. Table 1 summarizes similarities and differences between SAQM and CMAQ in terms of model inputs and building configurations.

Table 1. Similarities and differences between SAQM and CMAQ in model inputs and building configurations.

	SAQM	**CMAQ 4.4**
IDENTICAL		
Meteorol.	MM5 with HK observational nudging	
Emissions	HKEPD 2001 inventory database	
IC/BC	Initial/boundary conditions	
Diffusions	Horizon. – Briggs, Vert. – Eddies	
DIFFERENT		
Horizon. Advection	4^{th} Order Botts Scheme	Piecewise Parabolic
CB-IV	36 species, 83 reactions	45 species, 93 reactions

3. SIMULATION RESULTS

An O_3 episode was observed from 22 to 24 October 2003 over HK. High pressure system covering northern and eastern parts of China, together with typhoon KETSANA in the northwestern Pacific, bring air subsidence to HK, thus conducive to O_3 formation and buildup. The highest O_3 concentrations of 134.4, 126.2 ppb were recorded by HKEPD at Tung Chung station (TC, see Fig 2) on 22, 23 of October.

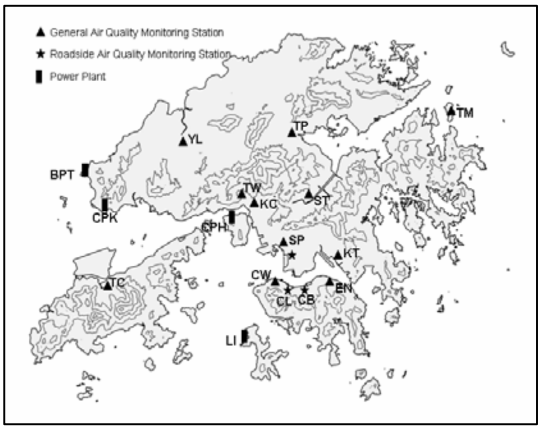

Fig. 2. HKEPD air quality monitoring stations. Topography also shown with contours at 200 m intervals.

3.1 Simulated MM5 fields

Applying FDDA to MM5 simulation, nudging with GTS reanalysis data in the 40.5 km resolution domain and with HKO observation data in the 1.5 km resolution domain, together with the update landuse data (Lo, 2004), results in better agreement (Huang, 2005). Spatial maps and wind vector time series can be referred to both of the works.

3.2 Simulated O_3

Both SAQM and CMAQ simulations covered 68 h from 0400 LST 22 October to 0000 LST 25 October 2003. Figure 3 displays time series of observed and simulated O_3 at various EPD air quality monitoring stations. TapMun (TM) locates northeastern part of HK and serves as a background site. While Central Western district (CW) represents the urban centre, Tung Chung (TC) reflects its proximity to the mouth of the PRD estuary and is adjacent to HK Airport. Simulated trends and peaks are similar at most places.

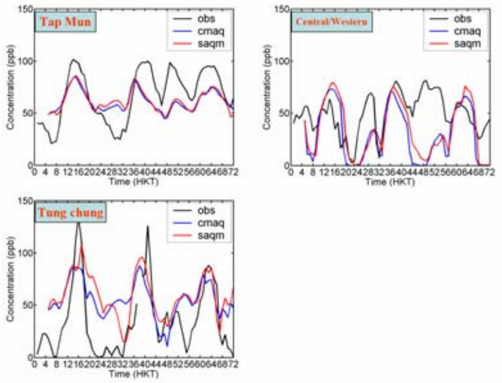

Fig. 3. Time series of O_3 at stations Tap Mun (MB), Central Western District (CW), and Tung Chung (TC), during the October 22, 2003 episode. Black: observation. Red: SAQM. Blue: CMAQ.

To facilitate further analysis of O_3 buildup, process analysis for both models is applied, which will be described in the next subsection.

3.3 Integrated Process Analysis

The idea is to break up the overall concentration into the contributing terms in the partial differential equations: horizontal advection, vertical transport, chemical production/loss, emissions, and wet/dry depositions. Detailed formulations are referred to Huang's (2005) work. Important processes are the horizontal advection (HADV), vertical transport (VTRA), chemical production/loss (CHEM), and dry depositions (DEPO), so our study will focus these four processes.

We choose the first and most severe day, October 22, 2003, pick the hours 9 am LST and 3 pm LST alone. For each of the bottom 11 sigma levels take the domain average for the innermost domain for each time slot. Then take the O_3 concentration difference between the afternoon and the morning. And we also take the difference for the HADV, VTRA, CHEM, and DEPO terms.

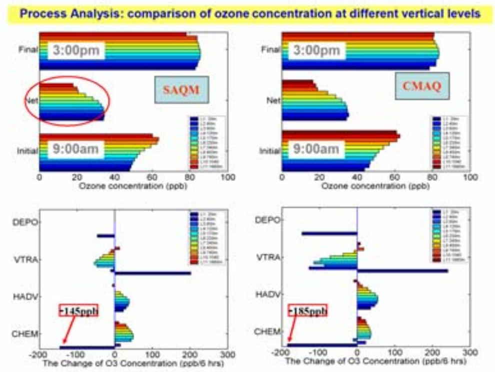

Fig. 4. Left top: SAQM O_3 concentration in 11 sigma levels at 9 am and 3pm LST, plus the difference. Left bottom: HADV, VTRA, CHEM, DEPO terms contributing to the concentration difference. Right top: as left top, except for CMAQ. Right bottom: as left bottom, except for CMAQ.

From Figure 4, the overall concentrations are similar in both models, in the aspects of vertical distribution and of magnitude order. So in both simulations around 35 ppb net O_3 have been produced at the surface layer. Similar patterns are observed in the individual terms in both models. For instance, chemistry terms are positive except at the surface, reflecting the loss due to titrations with species such as NOx at the surface, and production above surface due to photochemical reactions of O_2 and hydroxyl radical-related reactions. Horizontal advection brings in O_3 in both models in most layers. The gain due to vertical transport from just above surface implies that substantial portion of O_3 is imported from outside HK. Also note that the vertical transport term seems to serve as replenishment to the surface chemical loss. The fact that both models produce similar vertical profiles of processes may ascertain correct physical explanations to the production and buildup of O_3.

While the patterns in the individual terms are similar, larger magnitudes are produced in CMAQ. Table 2 displays the percentage difference in the process terms between CMAQ and SAQM.

Table 2. Percentage differences of process terms between CMAQ and SAQM (%)

Layer	DEPO	VTRA	HADV	CHEM
11	N/A	-100*	50*	-25*
10	N/A	1100*	100	-30
9	N/A	175*	93	-40
8	N/A	-500*	44	-48
7	N/A	2	40	-33
6	N/A	28	33	-43
5	N/A	43	20	-43
4	N/A	43	23	-28
3	N/A	97	30	120*
2	N/A	92	33	31
1(surf.)	67	15	24	22

* Magnitudes < 20 ppb

At surface layer, O_3 concentration is gained more in CMAQ than in SAQM through horizontal advection by 24% and vertical transport from above surface by 15%; the loss in CMAQ exceeds that in SAQM through chemical titration by 22% and dry deposition by 67%. The difference in CHEM term could be related to different CB-IV versions. More reactants and reactions seem to give rise to more O_3 loss.

For layers 3-5, the overall O_3 gain via horizontal transport in CMAQ exceeds that in SAQM by 31%, while at layer 2, O_3 loss due to vertical transport in CMAQ exceeds that in SAQM by 92%. So in CMAQ, much of O_3 in the intermediate layers is brought down to the surface. Only some is carried upward.

Loss is also contributed by the surface deposition term, which is more pronounced than in SAQM. This, together with the chemistry term, may contribute to under-prediction. Nonetheless, the process terms are similar qualitatively and give rise to similar net O_3 production.

4. SUMMARY AND CONCLUSION

SAQM and CMAQ were applied to investigate an ozone episode during October 22-24, 2003 in Hong Kong. Simulation of MM5 was improved with FDDA nudging and with update local landuse data. Simulation of SAQM and CMAQ was similar, especially in the net O_3 production. While similar O_3 vertical profiles of individual processes may ascertain correct physical explanations to the O_3 episode, magnitudes are more significant in CMAQ than in SAQM. The significant quantitative difference could be due to the difference in CB-IV versions used. Nevertheless, it is believed that CMAQ and SAQM are equally capable of simulating O_3 evolutions.

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