

USE OF CHEMICAL TRANSPORT MODEL FOR OZONE FORECAST IN TAIWAN

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ABSTRACT

An operational forecasting system using three-dimensional chemical transport photochemical model for predicting ground-level ozone concentrations in Taiwan has been developed. It consists of an emission model developed by Tamkang University, the mesoscale meteorological model RAMS, and the air quality model CAMx of Environ. In this paper, we introduce the component models, model coupling, and model initialization methods of this system. Then, the performance of this forecasting system during the 2002 ozone season were analyzed and discussed.

Key Words : real-time, Photochemical, Validation, RAMS, CAMx

1. INTRODUCTION

Ozone concentrations >120 ppbv have been observed relative frequently in Taiwan. Environmental Protection Administration of Taiwan have been forecasting next-day's pollutant standard index (PSI) since the year of 1992 to warn the public of unhealthy air and to encourage people to voluntarily reduce emissions-producing activities. Similar to Taiwan, many local authorities also issue air quality forecast in recent years. A lot of methods exist for forecasting ground-level ozone concentrations (USEPA, 2003). These methods can be classified into two categories, i.e., statistical and deterministic approaches.

The statistical models are based on the relations between a set of environmental predictors and the concentrations measured at different monitoring stations. Statistical approaches have been proposed for ozone forecasting include linear multiple regression, nonlinear regression, neural networks, classification and regression tree (CART). These approaches are easy to develop, however, there are systemic shortcomings that limit their usefulness. They require large training data sets for tuning the model's coefficients; hence they can be applied to regions with length observations only. The statistical models should be updated when emissions conditions change. This is a serious disadvantage in the circumstance of rapidly evolving primary pollutant emissions. In addition, high ozone episodes are rare events that may not be described properly by means of the classical statistical methods.

Deterministic models solve the governing equations that simulate the emission, transport, diffusion, transformation, and removal of air pollution to obtain the concentration distribution of ozone and other photochemical air pollutants. In the past, three-dimensional chemical transport models (CTM) have been widely used in air quality planning at different spatial scales in simulation mode (Russell and Dennis, 2000; Vautard et al., 2001). Currently, there is growing interest in the development of numerical air quality forecast systems by using CTM (McHenry et al., 1999; Chenevez and Jensen, 2001; Vaughan et al., 2004; CHRONOS, 2004). CTM approaches require numerous accurate input data (emissions, meteorology, land cover), which are difficult to collect in real time. This approach is difficult to develop and need large computer time to carried out the computations. In recent years, high performance computing at low cost has become available, so the latter problems should become less and less significant with time.

Although CTM have been widely used in Taiwan, this is the first time a numerical air quality forecasting system has been developed and validated in this island. In this paper, we will introduce this automated ozone forecast system and evaluate its performance.

2. BACKGROUND INFORMATION

Taiwan, which is lying between 23-25 N, and 121-123E, is an island located in the eastern side of Taiwan Strait. The topography of Taiwan, as shown in Fig. 1, is characterized by the ridge of Central Mountain. These mountains are steep with an altitude of 3000m and more and half width of few tens of kilometers. About 80% of the populations are live in the western side of Central Mountain. Taipei located in the northern Taiwan is the capital of Taiwan. Kaohsiung is an industrial city in the southern Taiwan.

The airflow in Taiwan is composed of both local and mesoscale wind system along with regional winds. Previous studies suggest that the local meteorology in Taiwan is controlled by several wind systems include the orographic blocking and barrier wind, land-sea breezes, mountain-valley winds, and urban heat island circulations. During summer time, Taiwan is dominated by subtropical high pressure of the Pacific Ocean and SW monsoon and typhoons; the latter two are often accompanied by high wind speed and unstable weather conditions, which are helpful for the dispersion of pollutants. The former, with its lower wind speed and high temperature, easily lead to higher concentrations of pollutants for the whole island. During winter time, Taiwan is dominated by NE wind. The Central Mountain acts as a barrier to the normal flow; a wake region will be developed on the downstream side (SW region of Taiwan). The solar radiations are strong and wind velocities are low at wake region so high ozone concentrations can occur even during early winter season.

As shown in Figure 1, Taiwan is divided into eight air quality forecast regions by Environmental Protection Administration of Taiwan. The geographical characters of each region are shown in Table 1.

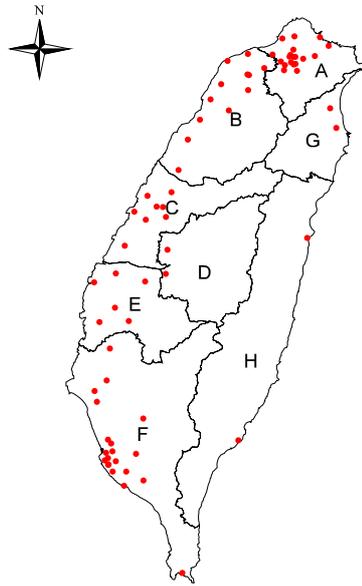


Figure 1. Locations of air quality forecast regions and air quality monitoring stations in Taiwan.

Table 1 Geographic characters of eight air quality forecast regions

Region	Counties	Characters
A	Keelung, Taipei	Urban areas with high population density and heavy traffic
B	Taoyuan, Hsinchu, Miaoli	Median size cities, industrial areas, rural area
C	Taichung, Changhua	Median size cities, rural area
D	Nantu	Foothills and Central Mountain
E	Yunlin, Chiayi, Tainan	Small cities, agriculture areas
F	Kaohsiung, Pingtung	Industrial region
G	Ilan	Lower developed agriculture region
H	Hualien and Taitung	Lower developed agriculture region

Figure 2 shows the time series of daily maximum 1h O₃ concentrations for eight ozone forecast regions in Taiwan based on the measured data obtained from 71 surface ozone monitor sites in Taiwan. In this figure, the regional daily maximum values are represented by the peak values from all stations if more than one monitor station are site within that area. As shown in this figure, the events of ozone concentrations >120 ppbv occur frequently in all regions except region G and H. The worst months for ozone concentration are May and October. From a regional perspective, the ozone problem in region A and region F are the worst. Region H (Hualien-Taitung) and Region G (Ilan) perennially post the nation's best air quality and poor air quality occurs at the most once a year.

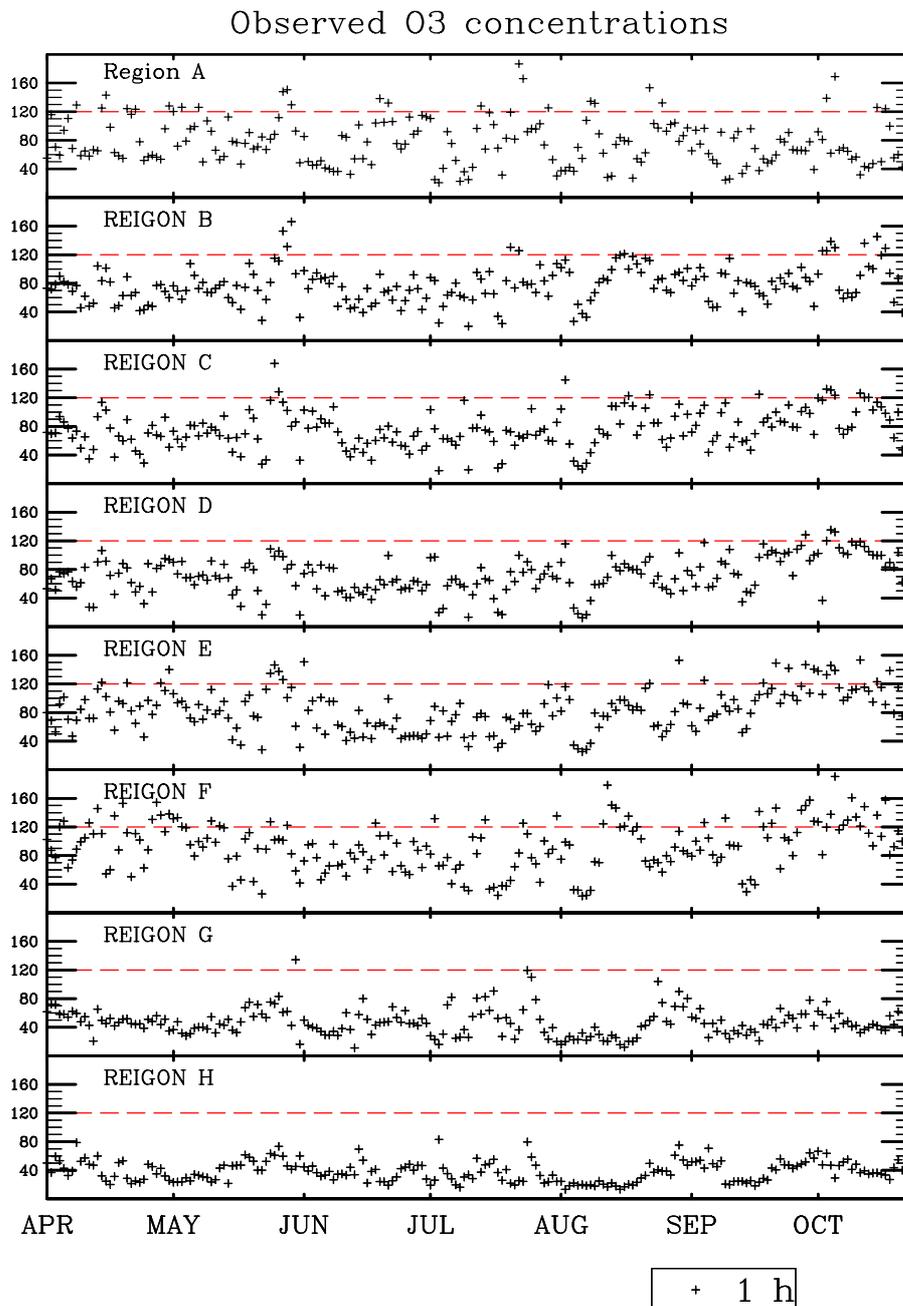


Figure 2. Daily maximum 1h O₃ concentrations for eight ozone forecast regions in Taiwan during ozone season of 2002.

3. METHODS

This forecast system consists of an emission processing model, a mesoscale meteorological model, and an air quality model. They were integrated to produce forecasts automatically.

The emission model is developed by Tamkang University. The emission data were obtained from three different organizations. The anthropogenic emission data in Taiwan were collected by CTCI and organized into a database called TEDS (Taiwan

Emission Data System). The biogenic emissions are estimated by using AVHRR data. The emission data outside Taiwan were obtained from Center for Global and Regional Environmental Research, University of Iowa (CGRER, 2002). Those data were merged and processed by a emission processing program developed by Tamkang University to generate the required input files for photochemical air quality model.

The meteorological model used in this study is RAMS developed by Colorado State University (Walko and Tremback, 1995). RAMS is running once every day, initialized at 18Z (02LST) and simulate for next 48 hours. Initial and boundary conditions are constructed after downloading AVN forecast file from the National Center for Environmental Prediction (NCEP). RAMS simulations using 3 nested-grids system. As shown in Fig. 3, the coarse (48km) domain covers much of East Asia. The second domain uses a uniform horizontal grid size of 12km. The very high-resolution 4km domain is centered on Taiwan, about 500km long and 300km wide. All RAMS domains use a polar-stereographic projection with 29 sigma-coordinate layers in the vertical.

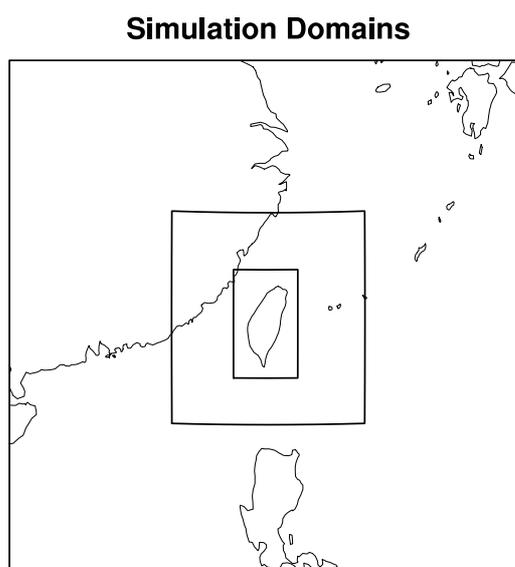


Figure 3. The nested grids used in meteorological simulations.

The photochemical air quality model used in this study is Comprehensive Air quality Model with extensions (CAMx) developed by Environ International (Environ International Co., 2002). CAMx is a 3-D Eulerian photochemical dispersion model. In this study, a modified version of the Carbon Bound IV chemical mechanism was used. The initial value problem is not of importance for the present study since the simulation is continuous. The initial conditions for next-day's simulation were determined from previous day's results. Clean tropospheric background concentrations were set on the boundary of coarse domain.

This system had operated in a real-time mode from April 1 to October 31, 2002. The results of forecast were saved for further analysis.

3. RESULTS AND DISCUSSION

(1) Forecasting results for daily maximum 1 h ozone concentrations

The results of day-to-day forecast have been evaluated against data obtained from 71 surface ozone monitor sites in Taiwan. Figure 4 shows the time series plots of observed and predicted daily peak 1-h ozone concentrations.

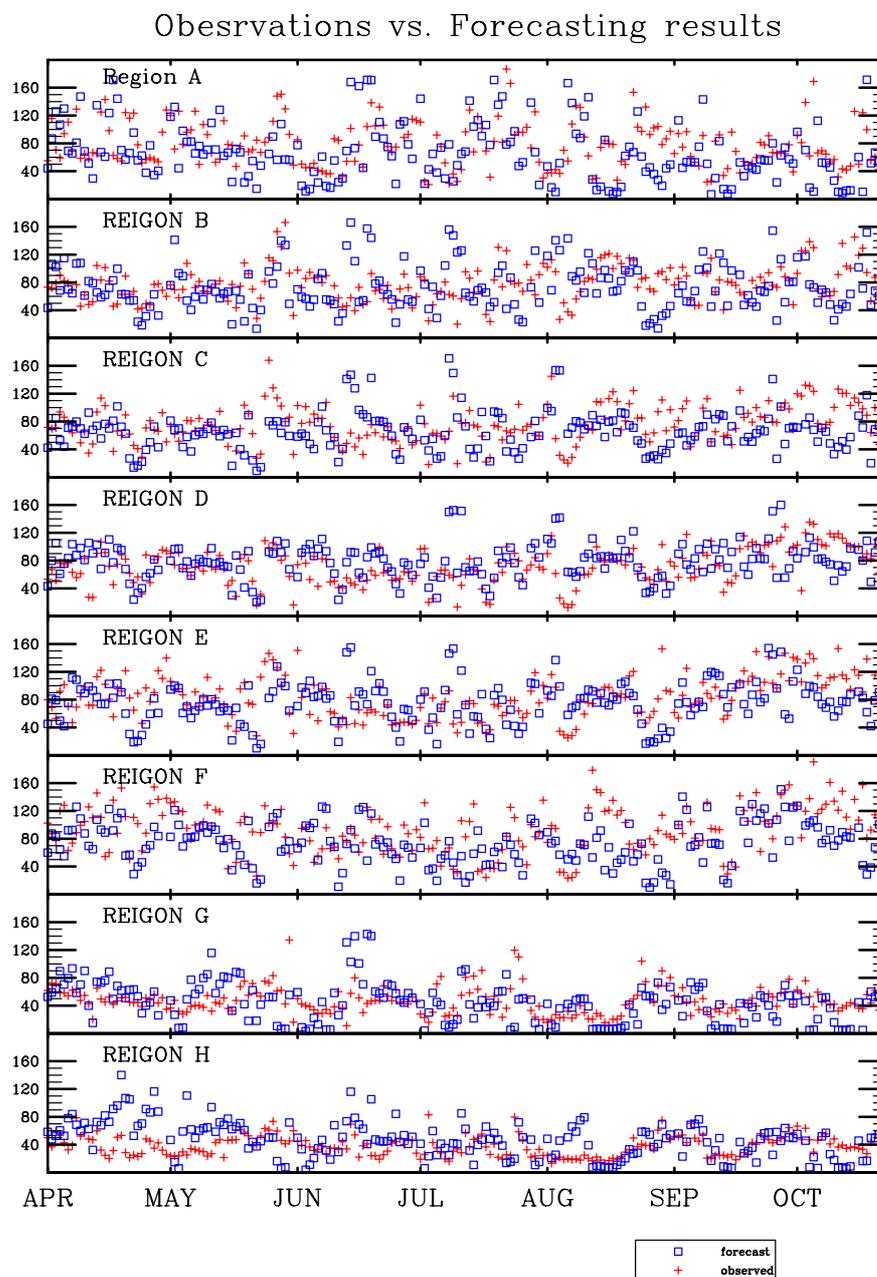


Figure 4. Time series plots of observed and predicted max. 1 h ozone concentrations.

Figure 5 shows the scatter plots of observed and predicted daily peak 1-h ozone concentrations for eight regions. The correlation coefficients (R^2) of observed and predicted concentrations are ranged from 0.12 to 0.41. From this prospect, the performance of this forecast system is not very satisfactory.

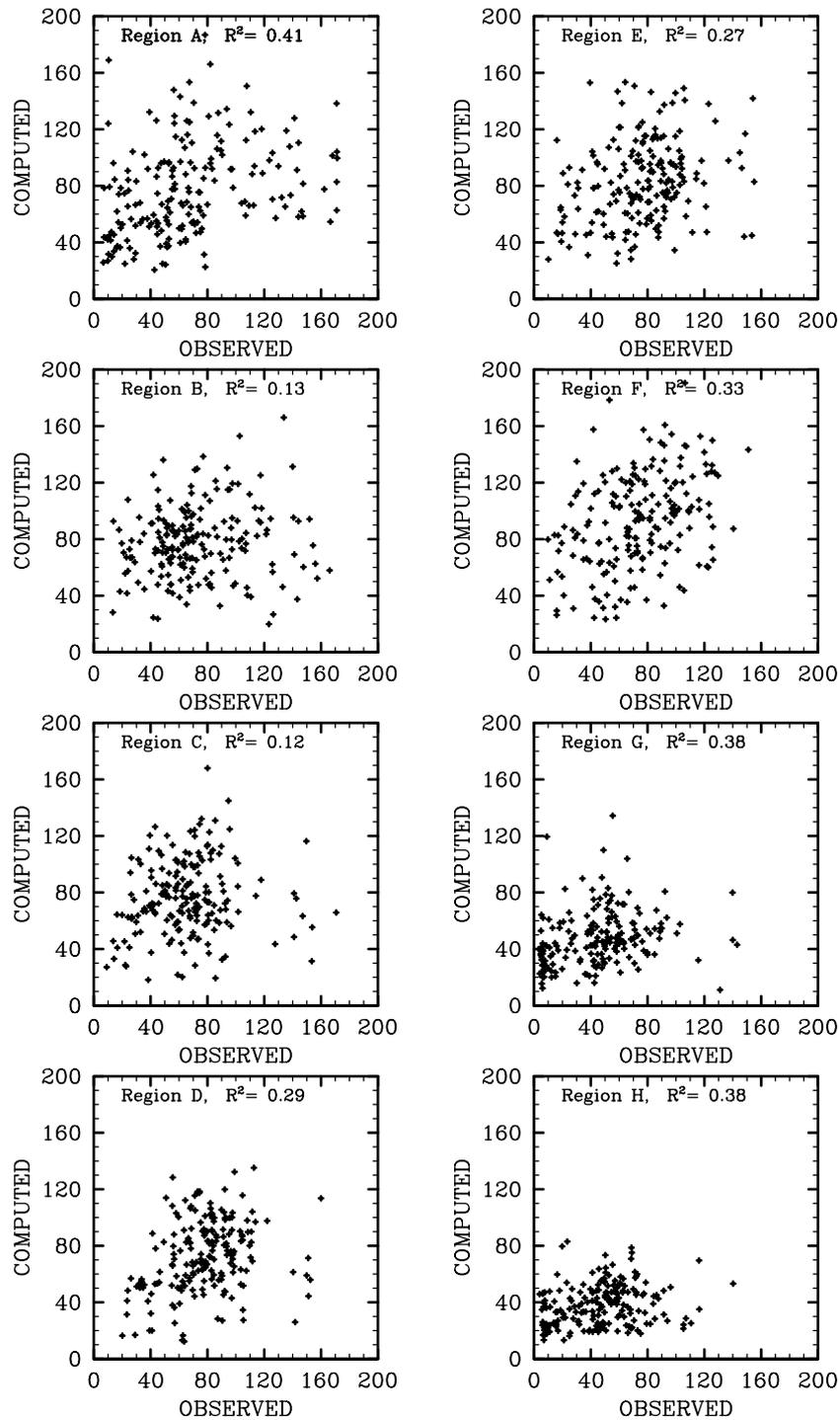


Figure 5. Scatter plots of observed and predicted max. 1 h ozone concentrations for eight regions during ozone season, 2002.

(2) Quantitative performance evaluation

Two different methods were used to evaluate the performance of this forecast system. The first approach is quite standard for model validation. The following measures were calculated for each monitoring station:

$$Bias = \frac{1}{N} \left[\sum_{i=1}^n (f_i - o_i) \right]$$

NB is Normalized Bias,

$$NB = \frac{1}{N} \left[\sum_{i=1}^n \frac{(f_i - o_i)}{o_i} \right]$$

MAE is mean absolute error,

$$MAE = \frac{1}{N} \left[\sum_{i=1}^n |f_i - o_i| \right]$$

In above equations, f denotes the daily peak 1-h ozone concentration for a specific stations, o is the corresponding ozone observed value. N is the number of samples which is equal to the number of stations in an air quality control area times the number of simulation days. This is a paired-in-space validation. The statistical summaries for 2002 simulation are shown in Table 1. The forecast is able to meet some performance criteria for regulatory models. Informal performance standards suggested by USEPA are: normalized bias ± 5 to $\pm 15\%$; normalized gross error ± 30 to $\pm 35\%$; unpaired peak prediction accuracy ± 15 to $\pm 20\%$.

Table 1. Paired-in-space validation for 2002 simulation

Region	AVE _s (ppb)	BIAS (ppb)	NB (%)	MAE (ppb)
A	60.50	-4.73	2.19	28.05
B	62.19	-7.03	-1.90	26.11
C	66.91	-8.31	-2.57	25.68
D	66.28	3.49	15.22	24.43
E	68.66	-5.99	1.33	24.96
F	72.31	-14.78	-11.57	29.87
G	49.72	-0.64	6.38	21.73
H	51.76	-3.33	-0.74	21.38

If the modeling targets switch to regional daily peak 1 h ozone concentrations, we will obtain the so called “regional validation”. The regional peak values are calculated as the average of the highest and second highest value in a specific region. The results of regional validation are shown in Table 2. Since the regional peak values were used, the average, bias and normalized bias values are increased.

Table 2. Regional validation for 2002 simulation

Region	AVE _p (ppb)	BIAS (ppb)	NB (%)	MAE (ppb)
A	76.89	-7.40	-3.74	33.89
B	76.43	-5.27	1.86	28.54
C	75.46	-9.47	-4.93	27.00
D	72.04	3.68	12.30	22.77
E	82.21	-6.91	-0.23	27.07
F	92.41	-15.58	-11.16	29.83
G	52.42	-2.65	1.69	20.72
H	53.31	-2.70	-3.15	16.67

Another method for verification of the ozone forecast utilizes a standard contingency table as shown in Table 3. As shown in this table, perfect forecast program would have values in cells "A" and "D" only. In the real world, imperfect forecasts result in values in cells "B" and "C".

Table 3. Contingency table for a two-category forecast

		Forecast	
		≥ 120ppb	<120ppb
observed	≥ 120ppb	A	B
	<120ppb	C	D

Table 4 shows a frequency table of the forecasted and observed events. It is constructed by counting the frequency of occurrence of each event and assigning it to the appropriate cell. In this table, the average of the highest and second highest value in a specific region were used for classification. The threshold values in Table 3 were changed to 100 ppb.

According to Table 4 the probabilities of detection (POD), which represents the percentage of ozone events that were correctly forecast, are less than 50%. False alarm rate (FAR) is greater than 50%. In order to maintain public confidence in the ozone forecast, it is desirable that the POD is reasonable high and the FAR should be reasonable low. From this point of view, the performance of this system is not good enough.

It worth to mention that small discrepancies in wind direction can produce significant shifts in the spatial pattern of predicted ozone concentration over a region. Taiwan is an island with steep mountains, a variety of mesoscale meteorological phenomena in the troposphere, including land-water circulation patterns, heat-island effect, and flows in complex topography all exert considerable influence on transport of air pollutants. Thus, many of the challenges associated with air quality forecasting for Taiwan are inherited from the difficulty in weather forecasting for this area. To accurately forecast the ozone concentrations in Taiwan is inherent a difficult task.

4. CONCLUSION

The system described here represents a new approach for ozone forecast in Taiwan. Although the performance of this system during the ozone season of 2002 is

reasonable, it is not accuracy enough to be used routinely by air quality managers. Since this system is so complex, there are numerous opportunities for improvements in the future.

Table 4. Frequency table for a two-category forecast

Region	(A)	(B)	(C)	(D)
A	9	30	25	115
B	6	22	24	135
C	1	27	9	145
D	2	12	18	142
E	8	38	17	123
F	27	40	19	89
G	0	2	2	97
H	0	0	2	118

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