

## Chapter 17

# Predicting Hourly Ozone Concentration Time Series in Dali Area of Taichung City Based on Seven Types of GM (1, 1) Model

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**Abstract.** In this study, seven types of first-order and one-variable grey differential equation model (abbreviated as GM (1, 1) model) were used to predict hourly ozone concentrations in Dali area of Taichung City, Taiwan. The results indicated that the minimum mean absolute percentage error (MAPE), mean squared error (MSE), root mean squared error (RMSE), and maximum correlation coefficient (R) were 19.00 %, 45.27, 6.73, and 0.91, respectively. All statistical values revealed that the prediction performance of GM (1, 1,  $x^{(0)}$ ), GM (1, 1, a), and GM (1, 1, b) is better than the performance of other GM (1, 1) models. The GM (1, 1) model required a very small sample size, as low as four samples, but the modeling could result in very high prediction accuracy. It is also revealed that GM (1, 1) GM (1, 1) was an efficiently early warning tool to provide ozone information to inhabitants.

**Keywords:** grey system theory, GM (1, 1), hourly ozone, air quality.

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## 1 Introduction

In the past two decades, air pollution has improved in most cities in Western Europe, North American as well as Japan. Air pollution reductions have resulted mainly from greater efficiency and pollution-control technologies in factories, power plants, and other facilities (Cunningham and Cunningham, 2006). Although improvements are also achieved in transportation, the regulation efficiencies of O<sub>3</sub> pollution sources are not as significant as those of other pollution sources because of their emitted and reactive characteristics (Faiz et al., 1995; Fischer et al., 2000; Kingham et al., 2000; Lipfert et al., 2006; Pai et al., 2007).

Among all air pollutants, the elevated O<sub>3</sub> concentrations at ground level are of particular concern, because of the harm to human health and vegetation. Gao and Niemeier (2008) indicated that ozone pollution was caused by photochemical reactions of precursor volatile organic compounds (often called non-methane hydrocarbons, NMHC) and nitrogen oxides, of which transportation emissions are the single major source. Several references showed that the mobile sources had a significant influence on ozone formation (Gao, 2007; Gao and Niemeier, 2007; Wang et al., 2009). In addition, the emissions of NMHC are one of the main contributors to ozone formation (Delucchi et al., 1994).

The relationship between ozone and its precursors is complicated due to the fact that meteorological and chemical reaction rates range from very fast to very slow. Such relationships between meteorological condition and ozone concentrations have been explored in several studies which have utilized statistical regression, graphical analysis, fuzzy theory, and cluster analysis.

Typically, environmental data are very complex for modeling because interrelations between various components result in a complicated combination of relations. Models providing reasonable accuracy have to consider physical and chemical relations among O<sub>3</sub> and other pollutants under various meteorological conditions simultaneously. However, the uncertainty problem will occur when above modeling approaches were adopted. One of the most important problems is the uncertainty of input data, including source identification, meteorological conditions, and relevant reaction mechanisms. No matter how good the inventory investigation was carried out in a large-scale modeling analysis, the uncertainties of input data in the mechanistic modeling process cannot be completely eliminated.

Many other attempts to model the interrelations have also been carried out. Linear regression methods, for instance, have been widely employed for decades (Abdul-Wahab et al., 2005). Additionally, to adequately model complex, non-linear phenomena and chemical procedures, artificial neural networks (ANN) and fuzzy logic approach have been widely applied because of their ability to model nonlinear data well (Gautam et al. 2008; Cai et al., 2009).

Although ANNs could predict air pollutant concentrations successfully, they require a large amount of training data. In order to simplify statistical complexity and gain consistent results from the investigation data for predicting air pollutant, the grey system theory (GST) offers a suite of methods.

The GST can resolve the problem of incomplete data and has been applied in our previous studies (Deng, 2002, 2005; Pai et al., 2007 a, b; Pai et al., 2008 a, b, c; Pai et al., 2010; Pai et al., 2010 a, b). GST focuses on the relational analysis, model construction, and prediction of the incomplete information. It requires only a small amount of data and the better prediction results can be obtained.

There are many methods of analysis in GST including grey model (GM). GM can be used to establish the relationship between many sequences of data. Among all air pollutants, the  $O_3$  concentrations at ground level are of particular concern because of the serious harm to human health, especially in a short-time period. If an efficient method could be developed to predict the short-time  $O_3$  concentrations, a better control strategy could be sought. Since the hourly data of particulate matter (PM) were predicted successfully using GM presented in our previous work (Pai et al., 2011), GM could be used to predict the hourly  $O_3$  concentrations.

The objectives of this study are as follows: (1) Construct seven types of first-order and one-variable grey differential equation model (abbreviated as GM (1, 1) model) for predicting hourly  $O_3$  concentrations in Dali area of Taichung City in Taiwan, (2) Compare the prediction performance of seven types of GM (1, 1) model.

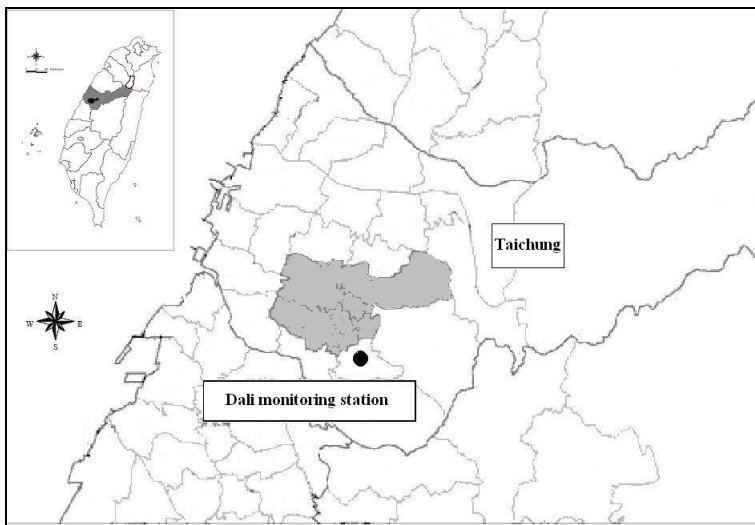
## 2 Materials and Methods

### 2.1 Data Set

The monitoring data from air quality monitoring station locating in Dali area of Taichung City was selected in this study (Figure 1). The concentrations of  $O_3$  from 29th of July to 16th of August 2008 were investigated. They were sampled and investigated every hour. The total number of data was 456. Among the data, 384 data points were used to estimate the coefficients of the models and 72 data points were used as the observed values when evaluating the performance of the model. The maximum, minimum, mean value and standard deviation of  $O_3$  series were 100.2, 1.1, 25.0, and 21.2 ppb, respectively. The meteorological condition was ignored in this study.

### 2.2 Grey Modeling Process

In a situation where information is lacking, using fewer (at least 4) system information, one can create a GM to describe the behavior of the few outputs. By means of accumulated generating operation (AGO), the disorderly and the unsystematic data may become exponentially behaved such that a first-order differential equation can be used to characterize the system behavior. Solving the differential equation will yield a time response solution for prediction. Through inverse



**Fig. 1** Dali area

accumulated generating operation (IAGO), the forecast can be transformed back to the sequence of original series. A grey modeling process is described as follows.

Assume that a series of data with  $n$  samples is expressed as:

$$X^{(0)} = (x^{(0)}(1), x^{(0)}(2), \dots, x^{(0)}(n)), \tag{1}$$

where the superscript  $(0)$  of  $X^{(0)}$  represents the original series. Let  $X^{(1)}$  be the first-order AGO of  $X^{(0)}$ , whose elements are generated from  $X^{(0)}$ :

$$X^{(1)} = (x^{(1)}(1), x^{(1)}(2), \dots, x^{(1)}(n)), \tag{2}$$

where  $x^{(1)}(k) = \sum_{i=1}^k x^{(0)}(i)$ , for  $k = 1, 2, \dots, n$ . Further operation of AGO can be conducted to develop the  $r$ -order AGO series,  $X^{(r)}$ :

$$X^{(r)} = (x^{(r)}(1), x^{(r)}(2), \dots, x^{(r)}(n)), \tag{3}$$

where  $x^{(r)}(k) = \sum_{i=1}^k x^{(r-1)}(i)$ , for  $k = 1, 2, \dots, n$ . The IAGO is the inverse operation of AGO. It transforms the AGO-operational series back to the one of a lower order.

The operation of IAGO for the first-order series is defined as follows:  $x^{(0)}(1) = x^{(1)}(1)$  and  $x^{(0)}(k) = x^{(1)}(k) - x^{(1)}(k-1)$  for  $k = 2, 3, \dots, n$ . After extending this representation to the IAGO of  $r$ -order series, we have

$x^{(r-1)}(k) = x^r(k) - x^r(k-1)$  for  $k = 2, 3, \dots, n$ . The tendency of AGO can be approximated by an exponential function. Its dynamic behavior resembles differential equation. The grey model GM (1, 1) thus adopts a first order differential equation to fit the AGO series,

$$\frac{dx^{(1)}}{dt} + ax^{(1)} = b \tag{4}$$

where the parameter  $a$  is the developing coefficient and  $b$  is the grey input. According to the definition, GM (1, 1) is that the order in grey differential equation is equal to 1 and defined as follows:

$$x^{(0)}(k) + az^{(1)}(k) = b \tag{5}$$

where  $z^{(1)}(k) = 0.5x^{(1)}(k-1) + 0.5x^{(1)}(k)$   $k = 2, 3, 4, \dots, n$ . Expanding (5), we have

$$\begin{aligned} x^{(0)}(2) + az^{(1)}(2) &= b \\ x^{(0)}(3) + az^{(1)}(3) &= b \\ \vdots &\quad \quad \quad \vdots \\ x^{(0)}(n) + az^{(1)}(n) &= b \end{aligned} \tag{6}$$

Transforming (6) into a matrix form, we have

$$\begin{bmatrix} x^{(0)}(2) \\ x^{(0)}(3) \\ \vdots \\ x^{(0)}(n) \end{bmatrix} = \begin{bmatrix} -z^{(1)}(2) & 1 \\ -z^{(1)}(3) & 1 \\ \vdots & \vdots \\ -z^{(1)}(n) & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} \tag{7}$$

Then the coefficients can be estimated by solving the matrix relationship,

$$p = \begin{bmatrix} a \\ b \end{bmatrix} = (B^T B)^{-1} B^T Y,$$

where  $p = \begin{bmatrix} a \\ b \end{bmatrix}$ ,  $B = \begin{bmatrix} -z^{(1)}(2) & 1 \\ -z^{(1)}(3) & 1 \\ \vdots & \vdots \\ -z^{(1)}(n) & 1 \end{bmatrix}$ , and  $Y = \begin{bmatrix} x^{(0)}(2) \\ x^{(0)}(3) \\ \vdots \\ x^{(0)}(n) \end{bmatrix}$ .

Sometimes, singularity would be encountered when treating the increasingly accumulated data. Then the inverse matrix could not be determined. Once this situation occurs, Computational Intelligence techniques could be applied. In this study, the increasingly accumulated data would not result in singularity due to their values and numbers were not too high. Additionally, the whitening type of GM (1, 1) model (or in terms of GM (1, 1, W)) that can be used for prediction is described as:

$$\hat{x}_1^{(1)}(k+1) = (x^{(0)}(1) - \frac{b}{a}) \cdot e^{-ak} + \frac{b}{a} \tag{8}$$

$$\hat{x}^{(0)}(k+1) = \hat{x}^{(1)}(k+1) - \hat{x}^{(1)}(k) \tag{9}$$

Additionally, there are several types of GM (1, 1) model which are derived from (4) as follows.

Connotation type of GM (1, 1): GM (1, 1, C)

$$x^{(0)}(k) = \left( \frac{1-0.5a}{1+0.5a} \right)^{k-2} \frac{b - ax^{(0)}(1)}{1+0.5a} \tag{10}$$

Grey difference type of GM (1, 1): GM (1, 1, x<sup>(1)</sup>)

$$x^{(0)}(k) = \beta - \alpha x^{(1)}(k-1) \tag{11}$$

where  $\beta = \frac{b}{1+0.5a}$  and  $\alpha = \frac{a}{1+0.5a}$ .

IAGO type of GM (1, 1): GM (1, 1, x<sup>(0)</sup>)

$$x^{(0)}(k) = (1 - \alpha)x^{(0)}(k-1) \tag{12}$$

Parameter-a type of GM (1, 1): GM (1, 1, a)

$$x^{(0)}(k) = \frac{1-0.5a}{1+0.5a} x^{(0)}(k-1) \quad (13)$$

Parameter-b type of GM (1, 1): GM (1, 1, b)

$$x^{(0)}(k) = \frac{x^{(1)}(k) - 0.5b}{x^{(1)}(k-1) + 0.5b} x^{(0)}(k-1) \quad (14)$$

Exponent type of GM (1, 1): GM (1, 1, e)

$$x^{(0)}(k) = x^{(0)}(3) e^{(k-3)\ln(1-\alpha)} \quad (15)$$

When adopting GM (1, 1,  $x^{(0)}$ ), GM (1, 1, a), GM (1, 1, b), and GM (1, 1, e),  $x^{(0)}(2)$  has to be calculated as follows:

$$x^{(0)}(2) = \beta - \alpha x^{(0)}(1) \quad (16)$$

All seven types of the GM (1, 1) model and their denotation are summarized in Table 1. The detailed derivation of these GM (1, 1) models can be found in Deng (2002, 2005).

### 2.3 Error Analysis

In order to evaluate the prediction accuracy of GM (1, 1), the mean absolute percentage error (MAPE), mean square error (MSE), root mean square error (RMSE), and correlation coefficient (R) were employed,

$$MAPE = \frac{1}{n} \sum_{i=1}^n \left| \frac{obs_i - pre_i}{obs_i} \right| \times 100\% \quad (17)$$

$$MSE = \frac{1}{n} \sum_{i=1}^n (obs_i - pre_i)^2 \quad (18)$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (obs_i - pre_i)^2} \quad (19)$$

**Table 1** Seven types of GM (1, 1) model

Type	Denotation	Prediction equation
Whitening type	GM (1, 1, W)	$\hat{x}_1^{(1)}(k+1) = (x^{(0)}(1) - \frac{b}{a}) \cdot e^{-ak} + \frac{b}{a}$
		$\hat{x}^{(0)}(k+1) = \hat{x}^{(1)}(k+1) - \hat{x}^{(1)}(k)$
Connotation type	GM (1, 1, C)	$x^{(0)}(k) = \left(\frac{1-0.5a}{1+0.5a}\right)^{k-2} \frac{b-ax^{(0)}(1)}{1+0.5a}$
Grey difference type	GM (1, 1, $x^{(1)}$ )	$x^{(0)}(k) = \beta - \alpha x^{(1)}(k-1)$
		$\beta = \frac{b}{1+0.5a}, \alpha = \frac{a}{1+0.5a}$
IAGO type	GM (1, 1, $x^{(0)}$ )	$x^{(0)}(k) = (1-\alpha)x^{(0)}(k-1)$
		$x^{(0)}(2) = \beta - \alpha x^{(0)}(1)$
Parameter-a type	GM (1, 1, a)	$x^{(0)}(k) = \frac{1-0.5a}{1+0.5a} x^{(0)}(k-1)$
		$x^{(0)}(2) = \beta - \alpha x^{(0)}(1)$
Parameter-b type	GM (1, 1, b)	$x^{(0)}(k) = \frac{x^{(1)}(k) - 0.5b}{x^{(1)}(k-1) + 0.5b} x^{(0)}(k-1)$
		$x^{(0)}(2) = \beta - \alpha x^{(0)}(1)$
Exponent type	GM (1, 1, e)	$x^{(0)}(k) = x^{(0)}(3)e^{(k-3)\ln(1-\alpha)}$
		$x^{(0)}(2) = \beta - \alpha x^{(0)}(1)$



$$R = \frac{\sum_{i=1}^n (obs_i - \overline{obs})(pre_i - \overline{pre})}{\sqrt{\sum_{i=1}^n (obs_i - \overline{obs})^2 \sum_{i=1}^n (pre_i - \overline{pre})^2}} \quad (20)$$

where  $obs_i$  is the observed value,  $pre_i$  is the result of prediction,  $\overline{obs}$  and  $\overline{pre}$  are the average values of observed values and prediction values, respectively.

### 3 Results and Discussion

#### 3.1 Determination of Grey Parameters

For determining the parameters of GM (1, 1), the observed O<sub>3</sub> data were plugged into (6) and the grey parameters were calculated by solving (7). When predicting, the values of the parameters a and b were equal to -0.00090492 and 23.404, respectively. According to (4), the parameter a (developing coefficient) will determine the predicting trend meanwhile parameter b (grey input) will determine the interception of (4).

#### 3.2 Simulation of O<sub>3</sub>

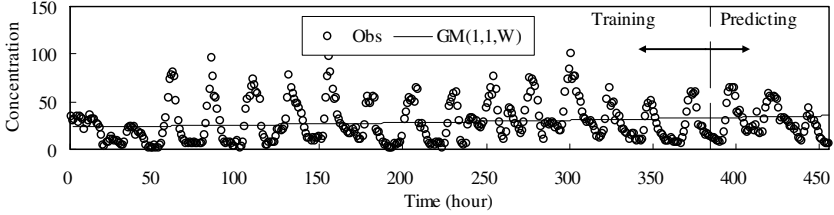
Table 2 shows all the values of MAPE, MSE, RMSE and R using seven types of GM (1, 1) model. The 1st to 384th data were used for constructing model, 385th to 456th data were used to evaluate the fitness. All values of the performance indexes revealed that the predicting performance of GM (1, 1, x<sup>(0)</sup>), GM (1, 1, a), and GM (1, 1, b) prevailed. Figure 2 (a), (b), and (c) depict the prediction results of O<sub>3</sub> using seven types of GM (1, 1) model.

As shown in Table 2, when constructing, MAPEs between the predicted and observed values of O<sub>3</sub> were between 29.03 % and 29.30 % using GM (1, 1, x<sup>(0)</sup>), GM (1, 1, a), and GM (1, 1, b), but they were 153.60 % - 220.96 % using other GM (1, 1) models. When predicting, the MAPEs were 19.00 % - 19.06 % when adopting GM (1, 1, x<sup>(0)</sup>), GM (1, 1, a), and GM (1, 1, b), but they were between 94.66 % and 147.43 % when using other GM (1, 1) models.

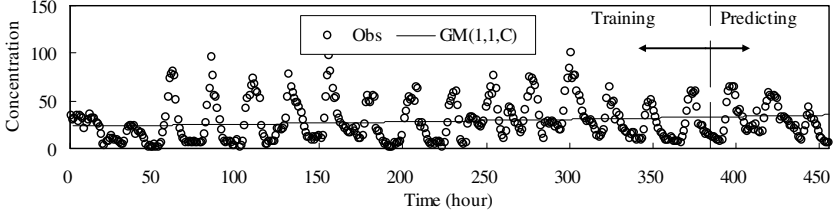
The MSE values of 78.85 - 79.48 using GM (1, 1, x<sup>(0)</sup>), GM (1, 1, a), and GM (1, 1, b) were lower than those of 440.64 - 541.01 using other GM (1, 1) models when model constructing. When predicting, the values of 45.27 - 45.41 using GM (1, 1, x<sup>(0)</sup>), GM (1, 1, a), and GM (1, 1, b) were also lower than those of 300.11 - 586.04 using other GM (1, 1) models. When constructing, the RMSE values of 8.88 - 8.92 using GM (1, 1, x<sup>(0)</sup>), GM (1, 1, a), and GM (1, 1, b) were lower than

**Table 2** The prediction performance for  $O_3$  using seven types of GM (1, 1) model

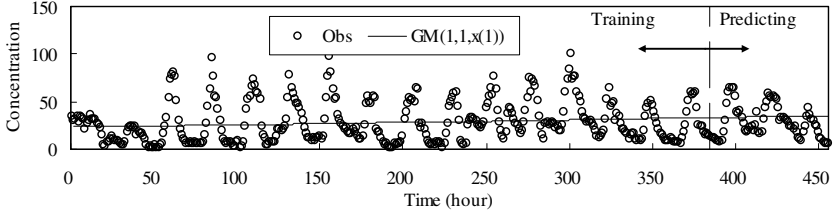
	MAPE		MSE		RMSE		R	
	Con-structing	Predict-ing	Con-struct-ing	Predict-ing	Con-struct-ing	Predict-ing	Con-struct-ing	Predict-ing
GM (1, 1, W)	154.46	95.40	440.64	302.28	20.99	17.39	0.14	-0.19
GM (1, 1, C)	154.30	95.28	440.64	301.93	20.99	17.38	0.14	-0.19
GM (1, 1, x(1))	153.60	94.66	441.07	300.11	21.00	17.32	0.13	-0.17
GM (1, 1, x(0))	29.30	19.06	79.48	45.41	8.92	6.74	0.91	0.91
GM (1, 1, a)	29.30	19.06	79.48	45.41	8.92	6.74	0.91	0.91
GM (1, 1, b)	29.03	19.00	78.85	45.27	8.88	6.73	0.91	0.91
GM (1, 1, e)	220.96	147.43	541.01	586.04	23.26	24.21	0.14	-0.19



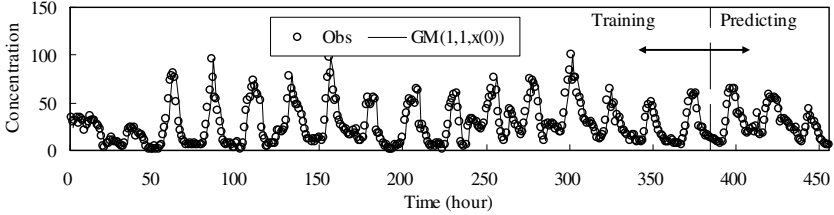
(a)



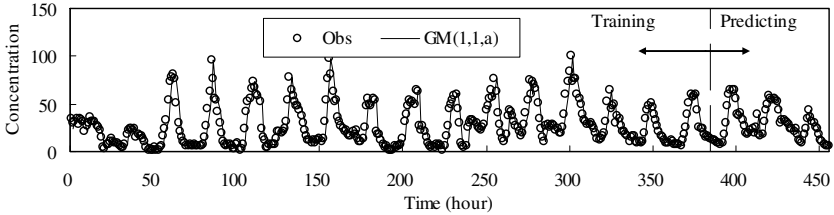
(b)



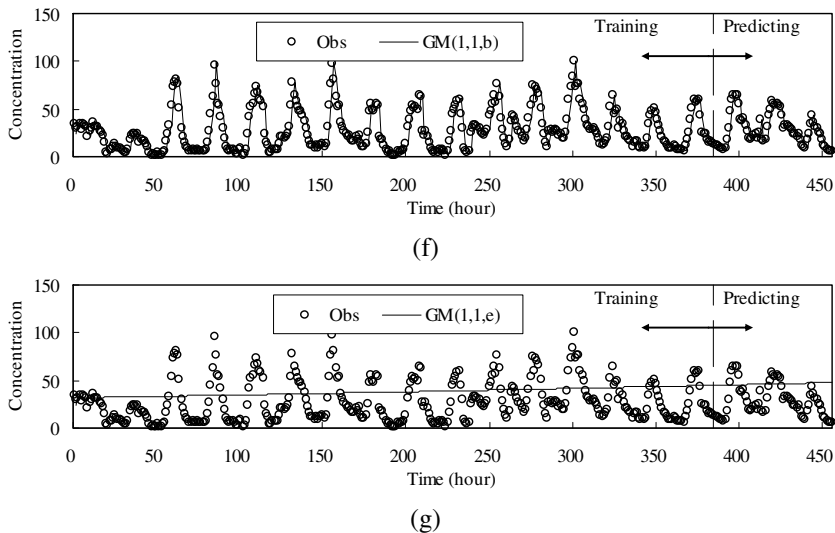
(c)



(d)



(e)



**Fig. 2** Prediction results of  $O_3$ , (a) GM (1, 1, W), (b) GM (1, 1, C), (c) GM (1, 1,  $x^{(1)}$ ), (d) GM (1, 1,  $x^{(0)}$ ), (e) GM (1, 1, a), (f) GM (1, 1, b), (g) GM (1, 1, e)

those of 20.99 – 23.26 using other GM (1, 1) models. The RMSE value of 6.73 – 6.74 using GM (1, 1,  $x^{(0)}$ ), GM (1, 1, a), and GM (1, 1, b) were also lower than those of 17.32 – 24.21 using other GM (1, 1) models when predicting.

When constructing, R value between the predicted and observed values of  $O_3$  was 0.91 using GM (1, 1,  $x^{(0)}$ ), GM (1, 1, a), and GM (1, 1, b), but they were 0.13 – 0.14 using other GM (1, 1) models. When predicting, the R was 0.91 when adopting GM (1, 1,  $x^{(0)}$ ), GM (1, 1, a), and GM (1, 1, b), but they were between -0.19 and -0.17 when using other GM (1, 1) models.

Comparable observations were similarly made by Abdul-Wahab et al. (2005). Abdul-Wahab et al. (2005) employed data on the concentrations of seven environmental pollutants ( $CH_4$ , NMHC, CO,  $CO_2$ , NO,  $NO_2$  and  $SO_2$ ) and meteorological variables (WS and direction, Temp, RH and solar radiation) to predict the concentration of ozone in the atmosphere using both multiple linear and principal component regression methods. They found that  $R^2$  for the day and night periods, were of 0.82 and 0.76, respectively. In this study, the R of 0.84 was obtained using GM.

Comparable observations were also made by Gautam et al. (2008). They proposed a new algorithm to predict the chaotic time series of  $O_3$  based on the ANN technique. They found that the MAPEs lay between 12.26 – 24.01 % using ANN and 9.46 – 13.55 % even using new algorithm.

In the study proposed by Cai et al. (2009), ANN was used to predict hourly air pollutant concentrations near urban arterials. The results indicated that the MAPE for predicting  $O_3$  fell in the range of 32.93 % and 45.15 %, RMSE were between 9.5 and 10.3, and R lay between 0.941 and 0.951, respectively.

In our previous study, seven types of GM (1, 1) models were used to predict hourly PM including  $PM_{10}$  and  $PM_{2.5}$  concentrations in Banciao City of Taiwan (Pai et al., 2011). The results indicated that the minimum MAPE, MSE, RMSE, and maximum R was 14.10 %, 25.62, 5.06, and 0.96, respectively when predicting  $PM_{10}$ . When predicting  $PM_{2.5}$ , the minimum MAPE, MSE, RMSE, and maximum R value of 15.24 %, 11.57, 3.40, and 0.93, respectively could be achieved. In this study, the minimum MAPE, MSE, RMSE, and maximum R was 19.00 %, 45.27, 6.73, and 0.91, respectively.

According to both results, the GM (1, 1) model required a very small sample size, as little as four sample points, however the modeling could result in very high prediction accuracy. Furthermore, the parameter estimation in GM (1, 1) model was only a procedure to fit a simple regression. Therefore, GM could be applied successfully in predicting  $O_3$  when the information was not sufficient.

In addition, the source identification, meteorological conditions, and relevant reaction mechanisms were taken as the input variables when using fuzzy or neural network models. But the source identification, meteorological conditions, and relevant reaction mechanisms did not be taken into account when using GM (1, 1). Although the mechanisms were unclear, the whitening part of the GM (1, 1) model could serve as useful reference to help observer realize more  $O_3$  variation.

## 4 Conclusions

Seven types of GM (1, 1) model were used to predict hourly  $O_3$  concentrations in Dali area of Taiwan. Their prediction performance was also compared. The conclusions can be drawn as follows. All statistical values revealed that the predicting performance of GM (1, 1,  $x^{(0)}$ ), GM (1, 1, a), and GM (1, 1, b) outperformed other models. When predicting  $O_3$ , the minimum MAPE, MSE, RMSE, and maximum R was 19.00 %, 45.27, 6.73, and 0.91, respectively. According to the results, it is shown that GM (1, 1) could predict the hourly  $O_3$  variation. Additionally, GM (1, 1) was an efficiently early warning tool for providing timely  $O_3$  information.

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