Quantification on source/receptor relationship of primary pollutants and secondary aerosols from ground sources—Part II. Model description and case study

Chien-Lung Chen, Ben-Jei Tsuang, Rong-Chang Pan, Chia-Ying Tu, Jen-Hui Liu, Pei-Ling Huang, Hsunling Bai, Man-Ting Cheng

Department of Environmental Engineering, National Chung-Hsing University, Taichung 40227, Taiwan, ROC

Institute of Environmental Engineering, National Chiao-Tung University, Hsin-Chu, Taiwan, ROC

Received 26 January 2001; received in revised form 12 September 2001; accepted 19 September 2001

Abstract

A Circuit Trajectory transfer-coefficient model (CTx) is developed in this study based on the parameterization presented in a companion paper (Tsuang et al., 2002). CTx was tested by applying it to Metropolitan Taipei for the entire year 1998. The model was calibrated in January and verified throughout the year. The results indicate that the correlation coefficients ($r$) for daily concentrations of CO, NOx, SO2, PM2.5 and PM10 were 0.75, 0.69, 0.39, 0.55 and 0.55, respectively, with biases of the means ranging from 0% to 20% during the verification period. According to contour plots of contributed concentrations to the city, “teleconnections” between source emissions and their contributions to the city can be identified. In addition, the model captures most of the dust episodes except during the periods of Asian dust storms. The sensitivity analysis shows that the calculated PM10 concentration is most sensitive to its dry deposition velocity as well as its emission rate. A more thorough study on the deposition velocity of PM2.5 is suggested. © 2002 Elsevier Science Ltd. All rights reserved.

Keywords: Transfer coefficient; Trajectory; Contributed concentration; Particulate matter; Sensitivity test; Taipei; Dust storm

1. Introduction

A Circuit Trajectory transfer-coefficient model (CTx) is developed in this study based on a theory for determining the transfer-coefficient presented in a companion paper (Tsuang et al., 2002). In the following sections, we describe the model structure and the parameterizations used in this model. Then, the model is applied to Metropolitan Taipei as a case study. Metropolitan Taipei is located in northern Taiwan, where rawinsonde data and intense surface meteorological data are continuously monitored and elevated sources are fewer in number. Hourly concentrations of CO, NOx, SO2, PM2.5 (particles whose sizes are < 2.5 µm in diameter) and PM10 (particles whose sizes are < 10 µm in diameter) are simulated and compared. In addition, we examine the sensitivity of calculated concentrations to a variety of model parameters and inputs. Then, we show that placing the emission rate in time series can improve the simulation in general. Finally, we discuss the application of the model for estimating the contributed concentrations of sources to Metropolitan Taipei during a PM10 episode day and a non-episode day.

2. Model description

2.1. Trajectories

In CTx, back-trajectories for a selected time (default 24 h) of transport were computed according to wind

*Corresponding author. Tel.: +886-4-22851206; fax: +886-4-22862587.
E-mail address: tsuang@nchu.edu.tw (B.-J. Tsuang).
data. There were three trajectories to the receptor (left, central and right). Each trajectory grid had a width of 10 km (i.e. Δy = 10 km). Trajectories were calculated using observed surface wind fields and adjusted to a selected height according to a log-vertical profile of wind speed. In addition, the minimum wind speed was set to be 1 m s⁻¹. The wind field along a trajectory was established in two steps: First, it was determined by the interpolation of observed wind data using the square of inverse-distance weighting method (US/EPA, 1994). Then, the interpolated wind field was further adjusted according to the channel effect of terrain (Scire et al., 2000; Tsuang et al., 2000). According to the weighting, the interpolated wind field along a trajectory was influenced most significantly by a nearby meteorological station data.

Once the trajectory paths were computed, the meteorological conditions along the path at each time step were extracted from the corresponding grid using the same interpolation method including air temperature, relative humidity, atmospheric pressure, wind speed, wind direction, cloud fraction, zenith angle and rain duration time.

2.2. Mixing height and stability

A Lagrangian model based on Tu (1999) is used to calculate the mixing heights and stabilities along the trajectory, where the land parameters are determined according to Tsuang and Tu (2001). Input data of relative humidity, pressure, wind vector, cloud fraction, zenith angle, rain duration time and lapse rate above a mixing height are used to run the sub-model. All the meteorological data were obtained by interpolating among the surface meteorological stations along the central trajectory, except for the lapse rate above a mixing height. Lapse rate above a mixing height is either set at a default value of the wet lapse rate (\(=−0.65\,\text{K km}^{-1}\)) or calculated according to rawinsonde data provided by users. The Lagrangian model parameterizes the mixing height according to Holzworth (1972).

2.3. Dry deposition, scavenging coefficient and gas–particle conversion rates

Similar to Lurmann et al. (1997), the dry deposition rates for gases were calculated based on a three-resistance dry deposition algorithm by Padro et al. (1991) and US EPA (1995), and those rates for all particles were calculated based on Slinn and Slinn (1980). Scavenging coefficients \(A\) for particle and \(SO_2\) were calculated by taking into account the precipitation rate according to Scott (1982), Kessler (1969), Seinfeld and Pandis (1998) and Uijlenhoet and Stricker (1999). The rest of gas scavenging coefficients for \(CO\) and \(NO_x\) were assigned as \(9.0\times10^{-12}\,\text{s}^{-1}\) and \(1.4\times10^{-10}\,\text{s}^{-1}\), respectively (Hertel et al., 1995). The gas–particle conversion rate of particulate sulfate from gaseous \(SO_2\) was set at \(5\%\,\text{Sh}^{-1}\) and that of particulate nitrate from \(NO_x\) was set at \(1.5\%\,\text{N}\,\text{h}^{-1}\) (Kuo et al., 1996). With respect to the size category of secondary aerosol, 85% of gaseous \(SO_2\) converted sulfate and 58% of gaseous \(NO_x\) converted nitrate are set to be in the radii of \(PM_{2.5}\) and the rests remain in \(PM_{2.5–10}\) according to the field data in a coastal area of Taiwan (Tsuang et al., 1999). The density of particulate matter is set to be \(2200\,\text{kg m}^{-3}\) (Juozaitis et al., 1996; Chate and Kamra, 1997). Parameters in the above references relevant to this study are listed in Table 1. The same parameters have been tested for the simulation of air pollutants with a Gaussian-type model in Taichung, where the measurements of sulfate aerosol and nitrate aerosol are available (Tsuang et al., submitted).

3. Taipei case study

Taipei City is the largest city in Taiwan. It has 2.6 million inhabitants. The population increases to 8.3 million people if the neighborhood counties of Taipei County, Keelung City and Taoyuan County are included (MOI, 2001). Taipei City is an ideal place in Taiwan to test the CTx model because the construction of new factories is not allowed and old factories were forced to relocate 20 years ago. Consequently, elevated sources are fewer in number. Note that the algorithm to calculate the transfer coefficients in CTx is valid only for ground sources.

Applying the model to Taipei City, we chose the air quality station at Ku-Ting as the receptor. The study period chosen was 1998, the first year when both the concentrations of \(PM_{10}\) and \(PM_{2.5}\) were measured and available simultaneously. Hourly concentrations of \(CO\), \(NO_x\), \(SO_2\), \(PM_{2.5}\) and \(PM_{10}\) at Ku-Ting station, measured continuously by the Environmental Protection Agency in Taiwan (EPA/ROC), were used in the study. Fig. 1 shows the location of the air quality station, the meteorological stations and the distribution of \(PM_{10}\) emissions rate used in the study. The region is characterized by complex terrain. Notable land–sea breezes, uphill–downhill winds and a monsoon climate cause significant diurnal and seasonal variability in weather conditions. In the winter, the prevailing wind comes from the northeast, and in the summer, the prevailing wind comes from the southwest. The initial concentrations of pollutants at the receptor for each month of the simulated period and the boundary condition for the concentrations at the beginning of the 24h trajectory were set at their observed values.
3.1. Emissions

Table 2 summarizes the emissions inventory in 1997 by CTCI (1999) in a region 10 km² and 30 km² centered at Ku-Ting station and four major stationary sources in the neighborhood counties. It shows that in the region of 10 km² and of 30 km² most of the pollutants, except SO₂, were dominated by ground sources, especially CO emissions. Up to 99% of CO emissions were from ground sources.

The emissions inventory by CTCI (1999) is only available in annual average. In order to take into account the day-of-the-week variability (DOWV), an index was introduced for parameterization of the short-term variability of emissions and especially the traffic (Ziomas et al., 1995; Simmonds and Keay, 1997; Cheng and Lam, 1998). The values of this index are presented in Table 3. The index was determined according to the DOWV of concentration levels at Ku-Ting station for the period 1994–1999. There is no significant difference in the values of the index from Monday to Saturday because of 6-day workweeks in Taiwan.

3.2. Meteorological data

Surface wind data were observed by either Central Weather Bureau (CWB/ROC) or EPA/ROC. Back-trajectories at 100 m height for 24 h of transport were computed according to the wind data. The temporal resolution of the observed wind data was 1 h and the spatial resolution was about 10 km. Since the temporal and the spatial resolutions of the wind data were much denser than those by Kahl and Samson (1986), Draxler (1987) and Rolph and Draxler (1990), the derived trajectories should be less problematic (Stohl, 1998).

---

Table 1

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle</td>
<td></td>
</tr>
<tr>
<td>Density&lt;sup&gt;a&lt;/sup&gt;</td>
<td>2200 kg m⁻³</td>
</tr>
<tr>
<td>Fine particle diameter (&lt;2.5 μm)</td>
<td>2.4 μm</td>
</tr>
<tr>
<td>Coarse particle diameter (2.5–10 μm)</td>
<td>4.5 μm</td>
</tr>
<tr>
<td>Scavenging coefficients</td>
<td></td>
</tr>
<tr>
<td>dry deposition velocity</td>
<td>Scott (1982)</td>
</tr>
<tr>
<td>Gas</td>
<td></td>
</tr>
<tr>
<td>SO₂ scavenging coefficients</td>
<td></td>
</tr>
<tr>
<td>Mass fraction between radii of 2.5 and 10 μm of SO₂ converted sulfate (f&lt;sub&gt;Sul&lt;/sub&gt;)&lt;sup&gt;b&lt;/sup&gt;</td>
<td>85%</td>
</tr>
<tr>
<td>Mass fraction between radii of 2.5 and 10 μm of NO&lt;sub&gt;x&lt;/sub&gt; converted nitrate (f&lt;sub&gt;Nit&lt;/sub&gt;)&lt;sup&gt;b&lt;/sup&gt;</td>
<td>58%</td>
</tr>
<tr>
<td>NO&lt;sub&gt;x&lt;/sub&gt; scavenging coefficients&lt;sup&gt;c&lt;/sup&gt;</td>
<td></td>
</tr>
<tr>
<td>CO scavenging coefficients&lt;sup&gt;d&lt;/sup&gt;</td>
<td></td>
</tr>
<tr>
<td>Gas–particle conversion rate of SO₂&lt;sup&gt;d&lt;/sup&gt;</td>
<td></td>
</tr>
<tr>
<td>Gas–particle conversion rate of NO&lt;sub&gt;x&lt;/sub&gt;&lt;sup&gt;d&lt;/sup&gt;</td>
<td></td>
</tr>
<tr>
<td>Dry deposition velocity</td>
<td></td>
</tr>
</tbody>
</table>

<sup>a</sup>Juozaitis et al. (1996), Chate and Kamra (1997).
<sup>b</sup>Tsai and Cheng (1999).
<sup>c</sup>Hertel et al. (1995).
<sup>d</sup>Kuo et al. (1996).

---

Fig. 1. Locations of the Ku-Ting monitoring station, Panchiao air sounding station, the largest PM₁₀ emission source (i.e. cement plant), the first three largest SO₂ emission sources (i.e. three coal-fueled power plants), two highways #1 and #3, meteorological stations (triangle) and distribution of PM₁₀ emission rate in the northern Taiwan. The rectangular area represents a region of 30 × 30 km² centered on Ku-Ting station.
Such a temporal resolution was able to capture the diurnal variation of wind direction in the study site. Lapse rate above a mixing height is obtained from rawinsonde data at Panchiao, about 9 km to the southwest and maintained by CWB/ROC.

3.3. Calibration

Since many parameters as well as the emission inventory are subject to particular uncertainties, calibration is usually necessary for applying air quality to a case study. We use the data of January 1998 for the calibration. Parameters calibrated by month will be applied to the rest of the year for the verification. First, we perform a sensitivity analysis to understand which parameters are the important parameters for the simulation. Sensitivity tests of the calculated concentrations to emission inventories, gas–particle conversion rates, dry deposition velocity, size fractions of gas converted second aerosols and scavenging coefficients are discussed (Chang et al., 1996; Jacobson, 1997b; Schwede and Paumier, 1997). The results are listed in Table 4. A sensitivity index SI in the table defined as (Yang et al., 1997)

\[
SI = \left( \frac{f(x + \Delta x) - f(x)}{f(x)} \right) / \left( \frac{\Delta x}{x} \right)
\]

is used to identify the key parameters, where \(x\) is one of the parameters, \(f(x)\) is the calculated result using the parameter \(x\), and \(\Delta x\) is a perturbation of \(x\). The larger the magnitude of the SI, the more important the parameter is. A negative SI indicates that the calculated concentrations decrease with the parameter. The table shows that the calculated \(\text{PM}_{10}\) concentrations are the most sensitive to the rate of the \(\text{PM}_{10}\) dry deposition velocity and then to the rate of the primary \(\text{PM}_{10}\) emission. Note that SI of the deposition rate is \(-118\%\) and that of the emission rate is \(91\%\). The \(\text{PM}_{10}\)
concentrations are less sensitive to the gas–particle conversion rates, the trajectory height and the size fraction of converted second aerosols. The magnitudes of the SIs of these parameters are <5%. Similarly, it is found that CO, NO\textsubscript{x}, SO\textsubscript{2} and PM\textsubscript{2.5} are most sensitive to their emission rates and dry deposition velocities. On rainy days, the scavenging coefficients of PM\textsubscript{10} and SO\textsubscript{2} are also important in determining their concentrations with SIs of about 12\%. In contrast, SIs of the scavenging coefficients of NO\textsubscript{x} and CO are about 0% and have little influence in determining their concentrations. Moreover, both the emission inventories (Tsuang and Chao, 1999; Chang et al., 2000; Kuang, 2000) and the dry deposition velocities over a complex terrain (Wesely and Hicks, 2000) are suspected of having of high uncertainty. Therefore, only these two dominant parameters are calibrated. Errors in the other terms are difficult to calibrate. However, Table 4 shows that they are not significant, and we do not calibrate them. It is worth knowing that these parameters alter mainly the magnitudes of the calculated concentrations with minor effects on improving the correlation coefficients. The correlation coefficients vary mainly with meteorological conditions and then with the variations of the emissions in time.

Next, we multiplied the dry deposition velocities calculated according to Wesely (1989) and Slinn and Slinn (1980) by a factor of 5, namely the exposure area ratio (EAR) of Metropolitan Taipei, in order to account for extra surfaces in Taipei for deposition. In urban areas, pollutants can be deposited on the sides of buildings in addition to roof surfaces. The current dry deposition schemes applied for complex terrain and urban areas are less reliable than those for flat areas (Wesely and Hicks, 2000). In addition to the EAR, the dry deposition rate for PM\textsubscript{2.5} has been further calibrated by doubling the rate according the result of another study site (Tsuang et al., 2001b). Note that the uncertainty of the dry deposition of the fine diameter has at least an order of magnitude (Seinfeld and Pandis, 1998). Finally, the emission rates of CO, NO\textsubscript{x}, SO\textsubscript{2}, PM\textsubscript{2.5} and PM\textsubscript{10} were scaled down by factors of 0.66, 0.63, 0.35, 0.91 and 0.41, respectively, to reach closer means of concentrations for each pollutant between observation and calculation during the calibration period. Table 5 summarizes the results of the simulations using the original and the calibrated parameters. No significant changes were found in the correlation coefficients but the biases have been reduced. The correlation coefficients of the calibration month for CO, NO\textsubscript{x}, SO\textsubscript{2}, PM\textsubscript{2.5} and PM\textsubscript{10} are 0.38, 0.53, 0.26, 0.49 and 0.54, respectively.

3.4. Verification

The calibrated emission inventory and dry deposition velocities are applied to February–December 1998 for verification. The results of the simulation are summarized in Table 6. The calculated and observed daily concentrations of CO and PM\textsubscript{10} are shown in Figs 2 and 3. They show that the simulations for CO, NO\textsubscript{x}, and SO\textsubscript{2} are satisfactory. No significant biases occur. The results indicate that the correlation coefficients (r) for daily concentrations of CO, NO\textsubscript{x}, SO\textsubscript{2}, PM\textsubscript{2.5} and PM\textsubscript{10}
were 0.75, 0.69, 0.39, 0.55 and 0.55, respectively. This shows that the simulated CO had the highest correlation and the simulated SO2 had the lowest correlation. The results are reasonable since, among these pollutants, CO had the largest portion of emissions from ground sources and SO2 had the lowest portion. Note again that the algorithms derived in the theory section are only valid for ground sources. Nonetheless, the table shows that the mean of PM2.5 concentrations was overestimated by 10 m/gm, particularly from May to August. At this stage, it is unclear which model errors caused errors in the response. One likely reason is that the dry deposition algorithm for particulates with size <2.5 μm is too low under light wind conditions. Note that in these months in Taipei, the mean wind speed was 2 m/s, and in the other months, the mean speed was 3 m/s.

An episode-distinguished ratio EDR is proposed here for evaluating the capability of a model in distinguishing between the episode and non-episode days. It is defined as

\[ \text{EDR} = \frac{\text{nos}}{\text{nos} + \text{noo} + \text{nou}}, \]  

where nos is the number of successful times in simulating the periods of episode days or non-episode days; noo is the number of non-episode days when the concentrations are overestimated as episode days; and nou is the number of episode days when the concentrations are underestimated as non-episode days. The episode day is defined as the day when the concentration is higher than the mean of the study period plus one standard deviation. The numerator of the EDR represents the number of successful predictions of the periods of episodes or non-episode days. The denominator of the EDR represents the total days of the prediction.

Table 6 shows that the model is capable of distinguishing between episode and non-episode days ranging between the episode and non-episode days. It is defined as

\[ \text{EDR} = \frac{\text{nos}}{\text{nos} + \text{noo} + \text{nou}}, \]  

where nos is the number of successful times in simulating the periods of episode days or non-episode days; noo is the number of non-episode days when the concentrations are overestimated as episode days; and nou is the number of episode days when the concentrations are underestimated as non-episode days. The episode day is defined as the day when the concentration is higher than the mean of the study period plus one standard deviation. The numerator of the EDR represents the number of successful predictions of the periods of episodes or non-episode days. The denominator of the EDR represents the total days of the prediction.

<table>
<thead>
<tr>
<th>Pollutant</th>
<th>Obs</th>
<th>Calc</th>
<th>Corr. coeff.</th>
<th>RMSE</th>
<th>Bias (%)</th>
<th>nos</th>
<th>noo</th>
<th>nou</th>
<th>noe</th>
<th>EAR/ ( a/(a + b + c) ) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO (ppm)</td>
<td>1.148</td>
<td>1.750</td>
<td>0.38</td>
<td>0.841</td>
<td>52.4</td>
<td>18</td>
<td>12</td>
<td>1</td>
<td>5</td>
<td>58</td>
</tr>
<tr>
<td>NOx (ppb)</td>
<td>57.4</td>
<td>90.6</td>
<td>0.53</td>
<td>40.7</td>
<td>57.8</td>
<td>17</td>
<td>14</td>
<td>0</td>
<td>5</td>
<td>55</td>
</tr>
<tr>
<td>SO2 (ppb)</td>
<td>3.7</td>
<td>10.6</td>
<td>0.26</td>
<td>8.0</td>
<td>186.5</td>
<td>8</td>
<td>23</td>
<td>0</td>
<td>7</td>
<td>26</td>
</tr>
<tr>
<td>PM2.5 (μg m(^{-3}))</td>
<td>38.6</td>
<td>46.2</td>
<td>0.52</td>
<td>14.3</td>
<td>19.7</td>
<td>21</td>
<td>7</td>
<td>3</td>
<td>7</td>
<td>68</td>
</tr>
<tr>
<td>PM10 (μg m(^{-3}))</td>
<td>51.1</td>
<td>76.2</td>
<td>0.54</td>
<td>36.2</td>
<td>49.1</td>
<td>22</td>
<td>9</td>
<td>0</td>
<td>6</td>
<td>71</td>
</tr>
<tr>
<td>CO (ppm)</td>
<td>1.148</td>
<td>1.156</td>
<td>0.38</td>
<td>0.446</td>
<td>0.7</td>
<td>23</td>
<td>4</td>
<td>4</td>
<td>5</td>
<td>74</td>
</tr>
<tr>
<td>NOx (ppb)</td>
<td>57.4</td>
<td>57.1</td>
<td>0.53</td>
<td>18.6</td>
<td>-0.5</td>
<td>25</td>
<td>1</td>
<td>5</td>
<td>6</td>
<td>81</td>
</tr>
<tr>
<td>SO2 (ppb)</td>
<td>3.7</td>
<td>3.7</td>
<td>0.26</td>
<td>2.2</td>
<td>0.0</td>
<td>23</td>
<td>1</td>
<td>7</td>
<td>7</td>
<td>74</td>
</tr>
<tr>
<td>PM2.5 (μg m(^{-3}))</td>
<td>38.6</td>
<td>38.5</td>
<td>0.49</td>
<td>11.2</td>
<td>-0.3</td>
<td>25</td>
<td>1</td>
<td>5</td>
<td>7</td>
<td>81</td>
</tr>
<tr>
<td>PM10 (μg m(^{-3}))</td>
<td>51.1</td>
<td>51.0</td>
<td>0.52</td>
<td>21.3</td>
<td>0.2</td>
<td>25</td>
<td>1</td>
<td>5</td>
<td>6</td>
<td>81</td>
</tr>
</tbody>
</table>

*a RMSE: root-mean-square error. Bias = (mean \( C_p \) − mean \( C_o \))/mean \( C_o \), where \( C_p \) and \( C_o \) are the predicted and observed concentrations. nos: number of successful times in simulating the periods of episode days or non-episode days, where the episode day is defined to be the day when the concentration is higher than the mean of the study period plus one standard deviation. noo: number of non-episode days when the concentrations are overestimated as episode days. nou: number of episode days when the concentrations are underestimated as non-episode days. noe: number of observed episode days. EDR: episode-distinguished ratio.

### Table 5

Statistics of original and calibrated daily CO, NO\(_x\), SO\(_2\), PM\(_{2.5}\) and PM\(_{10}\) concentrations in Taipei, Taiwan, January 1998

<table>
<thead>
<tr>
<th>Pollutant</th>
<th>Obs</th>
<th>Calc</th>
<th>Corr. coeff.</th>
<th>RMSE</th>
<th>Bias (%)</th>
<th>nos</th>
<th>noo</th>
<th>nou</th>
<th>noe</th>
<th>EAR/ ( a/(a + b + c) ) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO (ppm)</td>
<td>1.148</td>
<td>1.156</td>
<td>0.38</td>
<td>0.446</td>
<td>0.7</td>
<td>23</td>
<td>4</td>
<td>4</td>
<td>5</td>
<td>74</td>
</tr>
<tr>
<td>NOx (ppb)</td>
<td>57.4</td>
<td>57.1</td>
<td>0.53</td>
<td>18.6</td>
<td>-0.5</td>
<td>25</td>
<td>1</td>
<td>5</td>
<td>6</td>
<td>81</td>
</tr>
<tr>
<td>SO2 (ppb)</td>
<td>3.7</td>
<td>3.7</td>
<td>0.26</td>
<td>2.2</td>
<td>0.0</td>
<td>23</td>
<td>1</td>
<td>7</td>
<td>7</td>
<td>74</td>
</tr>
<tr>
<td>PM2.5 (μg m(^{-3}))</td>
<td>38.6</td>
<td>38.5</td>
<td>0.49</td>
<td>11.2</td>
<td>-0.3</td>
<td>25</td>
<td>1</td>
<td>5</td>
<td>7</td>
<td>81</td>
</tr>
<tr>
<td>PM10 (μg m(^{-3}))</td>
<td>51.1</td>
<td>51.0</td>
<td>0.52</td>
<td>21.3</td>
<td>0.2</td>
<td>25</td>
<td>1</td>
<td>5</td>
<td>6</td>
<td>81</td>
</tr>
</tbody>
</table>

### Table 6

Statistics of daily CO, NO\(_x\), SO\(_2\), PM\(_{2.5}\) and PM\(_{10}\) concentrations in Taipei, Taiwan, February–December 1998

<table>
<thead>
<tr>
<th>Pollutant</th>
<th>Obs</th>
<th>Calc</th>
<th>Corr. coeff.</th>
<th>RMSE</th>
<th>Bias (%)</th>
<th>nos</th>
<th>noo</th>
<th>nou</th>
<th>noe</th>
<th>EAR/ ( a/(a + b + c) ) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO (ppm)</td>
<td>1.099</td>
<td>1.147</td>
<td>0.75</td>
<td>0.276</td>
<td>4.4</td>
<td>282</td>
<td>27</td>
<td>17</td>
<td>54</td>
<td>87</td>
</tr>
<tr>
<td>NOx (ppb)</td>
<td>54.6</td>
<td>57.0</td>
<td>0.69</td>
<td>14.8</td>
<td>4.4</td>
<td>286</td>
<td>10</td>
<td>29</td>
<td>50</td>
<td>88</td>
</tr>
<tr>
<td>SO2 (ppb)</td>
<td>3.4</td>
<td>3.4</td>
<td>0.39</td>
<td>1.8</td>
<td>0.0</td>
<td>272</td>
<td>12</td>
<td>38</td>
<td>44</td>
<td>85</td>
</tr>
<tr>
<td>PM2.5 (μg m(^{-3}))</td>
<td>32.2</td>
<td>38.4</td>
<td>0.55</td>
<td>14.1</td>
<td>19.3</td>
<td>243</td>
<td>50</td>
<td>16</td>
<td>44</td>
<td>79</td>
</tr>
<tr>
<td>PM10 (μg m(^{-3}))</td>
<td>42.7</td>
<td>49.7</td>
<td>0.55</td>
<td>20.9</td>
<td>16.4</td>
<td>247</td>
<td>30</td>
<td>21</td>
<td>37</td>
<td>83</td>
</tr>
</tbody>
</table>
Fig. 2. CO daily concentrations at Ku-Ting station, Taiwan, 1998. (solid lines represent calculated concentrations and symbols observed data).
Fig. 3. PM$_{10}$ daily concentrations at Ku-Ting station, Taiwan, 1998. Arrows on the top of each graph represent Asia dust storm periods identified by Chang and Wu (2001). (solid lines represent calculated concentrations and symbols observed data).
from 79% to 88% varying with pollutants. The skills in CO, NO\(_x\), and SO\(_2\) are higher than PM\(_{2.5}\) and PM\(_{10}\). Most of the episodes occurred from November to April. The overestimation of the PM\(_{2.5}\) concentration in the summer deteriorates the EDR of PM\(_{2.5}\). With respect to PM\(_{10}\), the criterion of PM\(_{10}\) is its concentration higher than 66\(\mu\)g m\(^{-3}\). There were 44 PM\(_{10}\) episodes in 1998. The model captures 19 episodes but falsely reports 31 additional episodes. Most of the falsely reported episodes occurred under light wind conditions. With respect to the uncaptured 25 PM\(_{10}\) episodes, the periods of 12 of the 25 episodes (15–20 April, 17–18 October, 5 and 10 November, 8 and 15 December) corresponded with periods when Asian dust storms affected Taiwan. Fig. 3 also shows the periods identified by Chang and Wu (2001) when Taiwan was affected by Asian dust storms. The dust storms carry much dust of coarse radii (radii in the range 2.5–10\(\mu\)m) from desert regions in northern China. Transported long distances, they are known to subside over Taiwan during the synoptic weather pattern known as “a cold front passage”. The PM\(_{10}\) concentration consists of primary aerosol as well as secondary aerosol. To identify source–receptor relationship quantitatively, the back trajectories and contributed concentrations of PM\(_{10}\) are shown in Fig. 5a. The contributed PM concentration includes primary aerosol, sulfate, nitrate and ammonium. The open circles along the trajectory path indicate the directions and the locations of an air parcel at each hour. The stick on each of the circles shows the wind direction, and the small branches on the tail of a stick show its wind speed. The distance between two consecutive trajectory points is the distance wind traveled in 1 h. Shaded areas are the contributed concentrations of each grid in 1 \(\times\) 1 km\(^2\) resolution.

At 3 a.m., wind was nearly calm and circulated around Taipei Basin. The PM\(_{10}\) concentration was over 150\(\mu\)g m\(^{-3}\) in stable weather conditions and nocturnal inversion. The major contributed concentrations of PM\(_{10}\) came from nearby sources in Taipei City within the region of 10 \(\times\) 10 km\(^2\) centered on the receptor. They were mainly road dust and vehicle exhaust (CTCI, 1999). Highway 1, 20 km to the north, and one stationary source, Lin-Kou power plant, 25 km to the NWW from the receptor, were identified as major sources.

At 9 a.m., the air parcel entered Taipei Basin from the NW along a meandering trajectory to the receptor. The contributed concentrations along the trajectory in land were about 0.1–1\(\mu\)g m\(^{-3}\) km\(^{-2}\). Interestingly, the figure shows that sources in windward regions 7–11 h in advance of a receptor, where the wind speed was slow, had the highest contributed concentrations to the receptor. It shows a “teleconnection” between the source Highway 3, 20 km to the SWW, and the receptor. The contributed PM in this remote region was mainly nitrate aerosol converted from the emission of gaseous NO\(_x\) from the highway (Fig. 5b).

The back trajectories and contributed concentrations of CO are shown in Fig. 5c. In contrast to PM, the mechanisms involving the formation of CO only relate to the advection–diffusion mechanism. Unlike PM, there is no mechanism of transformation involved and no secondary CO exits. Hence, there is no “teleconnection” shown in the figure. The major contributed concentrations of CO came only from nearby sources in Taipei City within the region of 10 \(\times\) 10 km\(^2\) centered at the receptor—mainly vehicle exhaust.

4. Discussion

4.1. Source/receptor relationship

4.1.1. An episode day

On 8 January 1998, a PM episode occurred in which the daily average of PM\(_{10}\) was 92\(\mu\)g m\(^{-3}\), exceeding the criterion of 66\(\mu\)g m\(^{-3}\). This day belonged to the synoptic weather pattern known as “a cold front passage”. The PM\(_{10}\) concentration consists of primary aerosol as well as secondary aerosol. To identify source–receptor relationship quantitatively, the back trajectories and contributed concentrations of PM\(_{10}\) are shown in Fig. 5a. The contributed PM concentration includes primary aerosol, sulfate, nitrate and ammonium. The open circles along the trajectory path indicate the directions and the locations of an air parcel at each hour. The stick on each of the circles shows the wind direction, and the small branches on the tail of a stick show its wind speed. The distance between two consecutive trajectory points is the distance wind traveled in 1 h. Shaded areas are the contributed concentrations of each grid in 1 \(\times\) 1 km\(^2\) resolution.

At 3 a.m., wind was nearly calm and circulated around Taipei Basin. The PM\(_{10}\) concentration was over 150\(\mu\)g m\(^{-3}\) in stable weather conditions and nocturnal inversion. The major contributed concentrations of PM\(_{10}\) came from nearby sources in Taipei City within the region of 10 \(\times\) 10 km\(^2\) centered on the receptor. They were mainly road dust and vehicle exhaust (CTCI, 1999). Highway 1, 20 km to the north, and one stationary source, Lin-Kou power plant, 25 km to the NWW from the receptor, were identified as major sources.

4.2. Emission data and sounding data

There is always a request for a better data quality. Most frequently requested items include an emission inventory in time series and the availability of sounding data. Both of the data are relatively costly to procure. To evaluate their importance, the following tests are performed. First, we compare the calculated concentrations without using the DOWV in the emission inventory. The result is shown in Table 7, which shows that the model that took into consideration the DOWV of emissions improved the simulated results of the correlation coefficients. Second, we compare the calculated concentrations without using the sounding
Fig. 4. The ratios of PM$_{2.5}$ to PM$_{10}$ daily concentrations at Ku-Ting station, Taiwan, 1998. Arrows on the top of each graph represent Asia dust storm periods.
Fig. 5. Simulated (a) PM$_{10}$, (b) nitrate aerosol and (c) CO contributed concentrations on an episode day (8 January 1998). The receptor (solid circle) is Ku-Ting monitoring station. Contour lines represent the elevations.
data for estimating the mixing height. If there is no airsonde data, the lapse rate above mixing height is fixed to be the wet adiabatic lapse. Table 7 also shows the results of the model using wet adiabatic lapse rate instead of observed airsonde data. The correlation coefficient between simulated SO2 and observed data is worse. But, the results of PM10 are somewhat better than those results using airsonde data. Therefore, there is no significant improvement in using observed lapse rate than using wet lapse rate.

5. Conclusion

Although the current model is not as complete as some aerosol Eulerian models (Jacobson, 1997a,b; Lurmann et al., 1997; Nenes et al., 1999), the model is able to simulate the daily variation of PM concentration at a receptor. In addition, it is able to identify major sources of PM emission, SO2 emission and NOx emission contributing to the receptor with much smaller computational resources. The model takes cpu time of 263–367s, varying with output options, for 30 days of simulation on a Pentium II 350 running Red Hat Linux 6.0. In contrast to UAM aero2 using ISORROPIA code for aerosol simulation, it takes 37,477s of cpu time for 3 days of simulation over California’s south coast air basin on an HP 9000/715 workstation running HP-UX 9.05 (Nenes et al., 1999). The notion of determining transfer coefficients by an air quality model is important for the design of a better abatement strategy. The idea of determining transfer coefficients has been used for receptor models to determine low-cost strategies for the reduction of PM concentrations at receptors (Cass and McRae, 1983; Tsuang and Chang, 1997). This model determines the transfer coefficients qualitatively and quantitatively in the angular resolution as well as in the radial resolution.

The model results contrasted with observations in an air quality station in Taipei City indicate that the
correlation coefficient for daily concentrations of CO, NO\textsubscript{x}, SO\textsubscript{2}, PM\textsubscript{2.5} and PM\textsubscript{10} are 0.75, 0.69, 0.39, 0.55 and 0.55, respectively. Sensitivity analysis shows that the calculated concentrations are very sensitive to their dry deposition velocities. A more thorough study is suggested especially for that of PM\textsubscript{2.5}. Note that the above correlation coefficients can be compared with statistical models. Tsuang (1993) derived a multiple-linear regression equation to correlate PM\textsubscript{10} concentrations with meteorological factors with a correlation coefficient of 0.55 in Taipei. Ziomas et al. (1995) derived an equation to correlate daily maximum NO\textsubscript{2} concentration with meteorological factors and the previous day’s maximum concentration with a correlation coefficient of 0.68–0.72 in Athens, Greece.

It is therefore believed that the use of the model together with other prognostic systems can be used for air quality prediction and may enable the responsible authorities to issue warnings and take restrictive measures in advance. The priority regions where these restrictive measures can be taken are shown clearly on plots of the contributed concentration maps such as Figs 5 and 6 simulated by the model. This model is available to the public on the Internet at “http://air701.ev.nchu.edu.tw/ctx/” under the General Public License Agreements.

Acknowledgements

The author would like to acknowledge the support of this work by National Science Council, R.O.C., under contract NSC-88-2211-E005-018 and NSC-89-EPA-Z-005-004. Suggestions from Prof. Len-Fu W. Chang at Nat’l Taiwan Univ. are also appreciated.

References


CTCI Corporation, 1999. Carrying capacity management plan for air pollutants and estimation of emission inventory over Taiwan. Environmental Protection Administration, R.O.C.


Tsai, Y.I., Cheng, M.T., 1999. Visibility and aerosol chemical compositions near the coastal area in Central Taiwan. The Science of the Total Environment 231, 37–51.