Numerical Simulation of Photochemical Smog in Tokyo Metropolitan Area

by

Kiyohide Takeuchi* and Fujio Kimura

Meteorological Research Institute, Tokyo

(Received March 3, 1976)

Abstract

In order to clarify the mechanism of photochemical smog in the Tokyo Metropolitan Area, numerical simulation was performed. First, only dispersion was treated, by the use of sulfur dioxide (SO₂) and nitrogen oxides (NOₓ) as inert gas. And then photochemical smog was simulated by the dispersion model thus evaluated, combined with a photochemical reaction model.

The simulation model was developed in both Lagrangian and Eulerian forms, and case studies were carried out. In the Lagrangian approach (namely, moving parcel method), lateral diffusion was considered by “receptor-oriented method” and Friedlander and Seinfeld (1969) was used as a photochemical reaction model. In the Eulerian approach, calculation scheme MRI-E10 was developed for preventing “artificial diffusion” (see Appendix A), and the reaction model by Eschenroeder and Martinez (1971) and Sugiyama (1974) was utilized.

Generally speaking, results for SO₂ and NOₓ were fairly good. Simulation of the photochemical smog, however, was not so satisfactory yet. More information on the emission source (especially of hydrocarbon) in the area is indispensable, and a more practical model of the photochemical reaction in the atmosphere should be developed.

1. Introduction

In summer we suffer from the photochemical smog in many industrial and urban areas in Japan. The photochemical smog in our country is different in many respects from the well-known smog in the Los Angeles basin in the United States. For instance, nitrogen oxides (NOₓ) emitted from factories is generally significant in Japan, while in Los Angeles most of the NOₓ emission is mainly caused by automobiles.

Different models have recently been developed for simulating the photochemical air pollution (e.g., Friedlander and Seinfeld, 1969; Eschenroeder and Martinez, 1971). However, satisfactory results have not been obtained yet. In the Tokyo Metropolitan Area, the oxidant is one of the most serious problems, and a relatively sufficient set of data is available there, namely data on the source of emission, meteorological conditions and air quality. The aim of the present paper is to clarify the mechanism of the photochemical smog in this area.

First, we perform a provisional simulation on the primary pollutants for the purpose of evaluating both the model of source emission and the model of dispersion of pollutants in the atmosphere. For this simulation, sulfur dioxide (SO₂) and NOₓ are treated and considered as inert gas. The photochemical smog is then simulated by the use of the models thus evaluated, combined with a model of the photochemical reaction in the atmosphere.

There are two different viewpoints in fluid mechanics: namely Lagrangian and
Eulerian. We have developed the diffusion model in both Lagrangian and Eulerian forms.

2. Diffusion and photochemical reaction

2.1 Basic equation of diffusion

We have many models of numerical simulation for the atmospheric diffusion: plume model, puff model, box model and model using the diffusion equation. Each model has its own features, and so we have to choose one of them according to our aim. The plume and puff models are often used in Japan. The Climatological Diffusion Model, which is based on these models, plays an important role in the strategy making for abatement of the SO$_2$ concentration. However, CDM is not adequate to simulating the air pollution which is not stationary as in the photochemical smog. The box model cannot tell us about the fine distribution of concentration. On the other hand, the diffusion equation can treat both dispersion and photochemical reaction in the atmosphere, though it needs more time for computation. Survey of the study of the air pollution model in Japan is given elsewhere by one of the present authors (Takeuchi, 1976).

The diffusion equation comes from the conservation of mass of pollutants:

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} + V \frac{\partial C}{\partial y} + W \frac{\partial C}{\partial z} = \frac{\partial}{\partial x}(K_h \frac{\partial C}{\partial x}) + \frac{\partial}{\partial y}(K_v \frac{\partial C}{\partial y}) + \frac{\partial}{\partial z}(K_s \frac{\partial C}{\partial z}) + Q$$

(1)

where $C$ is the concentration, $(U, V, W)$ are the mean wind speeds along $(x, y, z)$ axes respectively, $K_h$ and $K_s$ are respectively the horizontal and vertical diffusivities, and $Q$ is the source intensity. The boundary condition is as follows:

$$K_s \frac{\partial C}{\partial z} = 0$$

at $z=0$ (ground surface), and $z=L$ (top of the mixing layer)

And

$$\frac{\partial C}{\partial x} = 0$$

at $x=0$ and $x_{max}$ (maximum $x$ in the area)

$$\frac{\partial C}{\partial y} = 0$$

at $y=0$ and $y_{max}$ (maximum $y$ in the area)

When we choose the coordinate system moving the air parcel, eq. (1) can be approximately written as:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}(K_s \frac{\partial C}{\partial z}) + Q$$

(4)

Here, we call eq. (4) a Lagrangian diffusion equation (see Fig. 1). We can then calculate the concentration of the pollutant at any receptor at any time, applying the equation to the parcel moving along the trajectory which arrives at the point specified. The parcel receives the pollutant during passing over the source.

![Fig. 1. Schematic diagram of Lagrangian model: air parcel parcel moving along the trajectory.](image-url)
2.2 Diffusion with photochemical reaction

The diffusion equation with the photochemical reaction is expressed in Eulerian form as

$$\frac{\partial C_i}{\partial t} + U \frac{\partial C_i}{\partial x} + V \frac{\partial C_i}{\partial y} + W \frac{\partial C_i}{\partial z}$$

$$= \frac{\partial}{\partial x} \left( K_x \frac{\partial C_i}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial C_i}{\partial y} \right)$$

$$+ \frac{\partial}{\partial z} \left( K_z \frac{\partial C_i}{\partial z} \right) + R_i + Q_i$$

Here, the suffix $i$ represents one of the species of pollutants, $R_i$ is the rate of formation of species $i$ by chemical reaction, and $Q_i$ is the rate of emission of species $i$ from the source.

In the Lagrangian approach, the following equation is applied to the air parcel

$$\frac{\partial C_i}{\partial t} = \frac{\partial}{\partial x} \left( K_x \frac{\partial C_i}{\partial x} \right) + R_i + Q_i$$

As is well recognized, photochemical reaction is so complicated in the atmosphere (e.g., Demarjian et al., 1974) that we cannot in practice take into account every possible reaction. A simplified model of the reaction, however, may often be good enough for the simulation in the atmosphere, considering the accuracy of other input data (e.g., Hanna, 1973).

3. Case study by Lagrangian simulation model

3.1 Simulation of SO$_2$

We choose July 31, 1972 for the Lagrangian simulation, because the meteorological condition (especially, the wind field in the area) was rather simple and the set of data was nearly sufficient. Fig. 2 shows the trajectory reaching Urawa City, Saitama Pref. at 1600JST, which was determined from the hourly made streamline on the surface.

We took into account the shaded area in the figure, in which the source of SO$_2$ emission made a contribution to the parcel arriving at the City: namely, we applied "receptor-oriented method". Here, the area was determined in such a way that the width of ($\sigma_y + 500$ m) was taken on both sides of the trajectory; $\sigma_y$ is the standard deviation of the plume under the slightly unstable condition in the atmosphere (see, e.g., Turner, 1970) and the initial spread of the pollutant is expressed by the additional width of 500 m. Thus, we considered the lateral diffusion of the pollutant.

The source intensity here used is based on the data of the stationary source which the local authorities recently surveyed. The source was categorised into three classes according to its effective height which was calculated after the CONCAWE equation (developed by "Conservation of Clean Air and Water, Western Europe" Group: see Brumage, 1968). The source intensity in the shaded area is shown in Fig. 3. We find there that the source is concentrated in the Kawasaki industrial area.

We used the vertical diffusivity of 20 m$^2$/s suggested by Sato (1975). The mixing height was obtained from the lower tropo-
spheric radiosonde.

We solved eq. (4) with our calculation scheme called MRI-L10. The vertical grid size of 25 m was taken for calculation. The surface concentration thus calculated is shown in Fig. 4. The result shows that we overestimated the concentration. It might be because we neglected the increase of wind speed with height. Actually, the wind speed observed by the pilot balloon was 9.5 m/s at a height of 300 m, while the surface wind was 4.0 m/s at Setagaya at 1400JST.

![Fig. 3. Sources of the SO₂ emission along the trajectory.](image)

3.2 Simulation of photochemical smog

Since we do not have reliable information on the emission of hydrocarbon (HC), no sophisticated model of photochemical reaction can work well. Therefore, we adopted the simplified model presented by Friedlander and Seinfeld (1969) and used the observed concentration of HC.

Finally the reaction model can simply be expressed as follows.

The concentration of HC:

\[ [\text{HC}] = \text{const.} \]

(the observed concentration)

The rate of formation of NO₂:

\[ R_{\text{NO}_2} = -[\text{NO}] [\text{HC}] (\alpha[\text{NO}] - \lambda[\text{NO}_2]) \]

The rate of formation of NO:

\[ R_{\text{NO}} = -[\text{NO}_2][\text{NO}][\text{HC}] \]

The concentration of ozone O₃:

\[ [\text{O}_3] = \beta[\text{NO}_2]/[\text{NO}] \]

Here, \( \alpha, \beta \) and \( \lambda \) are constants to be determined empirically.

The stationary source of NOₓ was estimated in a similar way to that of SO₂. On the other hand, the mobile source was presented by 2 km mesh as a function of time, based on the traffic data which the local authorities recently gathered. And it was assumed that nitric oxide (NO) and nitrate dioxide (NO₂) were emitted into the parcel at the same rate from the source, both stationary and automobile, because the observed concentration of NO was almost the same as that of NO₂ on the preceding night. The results were not so good (see Fig. 5). The reasons of disagreement may be as follows:
(1) in our simulation comparison should be made only near the end point of the trajectory; (2) the initial concentration of pollutants except HC was neglected, and it might greatly affect the ozone concentration due to nonlinearity of the reaction model; (3) since the reaction model is too simple to be applicable to the wide range of concentration as in the atmosphere. For instance, in the present model the reaction rate becomes much lower when the concentration is low.

4. Case study by Eulerian simulation model

4.1 Simulation of SO$_2$ and NO$_x$

The Eulerian simulation model is very powerful to obtain the variation of the concentration in time and space. For simplicity we assumed that the wind velocity was only a function of the height and the time in our scheme of computation, MRI-E10 (see Fig. 6 and Appendix A).

The computational area (60 km $\times$ 60 km) covered the central part of the Metropolitan Area, and the mesh size was 2 km $\times$ 2 km $\times$ 100 m (height). The stationary source was treated in a similar way to the Lagrangian case. As for the automotive source, we followed the pattern of weekday traffic in the area. Figs. 7 and 8 show respectively the stationary and the automotive source of NO$_x$ emission.

Simulation was performed for July 26, 1973, which was a typical summer day covered with the anticyclone. The mixing height and the vertical diffusivity were determined in a similar way as in the previous section; the diffusivity suggested by Sato (1975) was obtained from the nonlift balloon observation on the same day. The horizontal diffusivity was assumed to be proportional to the vertical (the constant of proportionality was here taken to be five). Figs. 9 and 10 show the mixing height and the wind profile which were used as input data.

The concentrations of SO$_2$ and NO$_x$ are respectively shown in Figs. 11 and 12, where the numeral in a circle indicates the observed value. Agreement is fairly good, though the NO$_x$ concentration in the west part of the area is underestimated and both concentrations near the big source are overestimated. It may be because we neglected the source of emission in Yokohama City,
Fig. 7. Source intensity of stationary NO$_x$ emission in the Tokyo Metropolitan Area.

Fig. 8. Source intensity of automotive NO$_x$ emission.

Fig. 9. Variation of the mixing height which was determined from the lower tropospheric radiosonde on July 26, 1973.
Fig. 10. Time sequence of wind profile which was obtained from pilot balloon observation at several sites in the area on July 26, 1973.

Fig. 11. SO₂ concentration at the ground surface: calculated (solid line) and observed (in circle).
Kanagawa Pref., located in the south of the area, and because our mesh size was too large to make accurate simulation of the diffusion near the big point source.

4.2 Simulation of photochemical smog

Since the results of our simulation for inert gases such as SO$_2$ and NO$_2$ were not bad, we proceeded to make simulation of the photochemical smog in the same area. Since the reaction model used in the Lagrangian model has the shortcoming mentioned above, we used the model presented by Sugiyama (1974) (see Table 1). He has improved the model by Eschenroeder and Martinez (1971) for the purpose of saving the computing time and securing better fitting to the chamber experiment.

The formation rate of species $i$, $R_i$ in eq. (5) is given in Table 1. The concentration was calculated for NO, NO$_2$, HC and O$_3$, on the assumption of a quasi-stationary state for O, OH, RO$_2$ and HNO$_2$. Some detailed

Table 1. Photochemical reaction model (Sugiyama, 1974)

<table>
<thead>
<tr>
<th>No.</th>
<th>Reaction</th>
<th>Rate constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$h\nu + NO_2 \rightarrow NO + O$</td>
<td>0.52 min$^{-1}$</td>
</tr>
<tr>
<td>2</td>
<td>$O_2 + O_3 + M \rightarrow O_3 + M$</td>
<td>$1.31 \times 10^{-5}$ ppm$^{-1}$ min$^{-1}$</td>
</tr>
<tr>
<td>3</td>
<td>$O + NO \rightarrow NO_2 + (O_2)$</td>
<td>6 ppm$^{-1}$ min$^{-1}$</td>
</tr>
<tr>
<td>4</td>
<td>$O + HC \rightarrow 2RO_2$</td>
<td>2000 ppm$^{-1}$ min$^{-1}$</td>
</tr>
<tr>
<td>5</td>
<td>$OH + HC \rightarrow 2RO_2$</td>
<td>80 ppm$^{-1}$ min$^{-1}$</td>
</tr>
<tr>
<td>6</td>
<td>$RO_2 + NO \rightarrow NO_2 + 0.5 OH$</td>
<td>800 ppm$^{-1}$ min$^{-1}$</td>
</tr>
<tr>
<td>7</td>
<td>$RO_2 + NO_2 \rightarrow PAN$</td>
<td>6 ppm$^{-1}$ min$^{-1}$</td>
</tr>
<tr>
<td>8</td>
<td>$OH + NO \rightarrow HNO_2$</td>
<td>20 ppm$^{-1}$ min$^{-1}$</td>
</tr>
<tr>
<td>9</td>
<td>$OH + NO_2 \rightarrow HNO_3$</td>
<td>100 ppm$^{-1}$ min$^{-1}$</td>
</tr>
<tr>
<td>10</td>
<td>$O_3 + HC \rightarrow RO_2$</td>
<td>0.03 ppm$^{-1}$ min$^{-1}$</td>
</tr>
<tr>
<td>11</td>
<td>$(H_2O +)NO + NO_2 \rightarrow 2HNO_2$</td>
<td>0.001 ppm$^{-1}$ min$^{-1}$</td>
</tr>
<tr>
<td>12</td>
<td>$h\nu + HNO_2 \rightarrow NO + OH$</td>
<td>0.13 min$^{-1}$</td>
</tr>
</tbody>
</table>

Note M : any third body
RO$_2$: free radical
description is given in Appendix B. Furthermore, PAN and HNO$_3$ were removed from the system considered.

Though the model is sensitive to the initial concentration of HC, we have very poor information available on HC. We took into account HC emitted only from automobiles and assumed that the initial concentration of HC (at 0700JST) was 0.2 ppm and NO$_2$ was emitted at the rate of 1/3 of NO (considering the mesh size, the initial concentration of automotive exhaust gas and the vertical diffusion). Other input for the calculation was the same as before.

The surface distribution of oxidant concentration thus obtained is shown in Fig. 13. Fig. 14 indicates the time change of the concentrations. Our calculation starts at 0700JST, but a comparison is made from 1000JST between the calculated concentrations and the observed ones. It is because results in the first several hours will be much affected by the initial concentration we adopted. The vertical distribution of the concentrations is also depicted in Fig. 15, where the observed value was obtained with a tethered balloon.

The calculated concentration of oxidant is generally underestimated, but it has a similar feature to the observed one.

5. Discussion and concluding remarks

Our simulation model in the Tokyo Metropolitan Area showed fairly good agreement for inert gases such as SO$_2$ and NO$_2$. However, the results of simulation of the photochemical smog was not satisfactory: namely, our models can make a simulation qualitatively but still have many difficulties in the quantitative sense. It may be mainly due to poor data on hydrocarbon.

The oxidant concentration depends on the initial concentration of hydrocarbon, [HC]$_0$ and on the ratio of emission rate between NO and NO$_2$, $Q_{NO}/Q_{NO_2}$. Table 2 gives some examples of dependency of the oxidant concentration upon combination of [HC]$_0$ and $Q_{NO}/Q_{NO_2}$. Case A is what was adopted in this paper. The oxidant concentration in case B where $Q_{NO}/Q_{NO_2}$=19, decrease by 30–40 percent compared with case A. Cases C and D are the case where [HC]$_0$ is different from case B. The oxidant concentration especially in case D where [HC]$_0$ =0 becomes about one order of magnitude lower than cases B and C. This implies that the initial concentration of hydrocarbon has much effect on the oxidant concentration, and that the emission rate of hydrocarbon here used might be underestimated.
Fig. 14. Time variation of the concentration (NO, NO₂ and O₃).

Fig. 15. Vertical distribution of the concentration (NO, NO₂ and O₃).
Accumulation of reliable information on the pollutants (especially on hydrocarbon) is urgent, and a more practical model of the photochemical reaction in the atmosphere should be developed. It is a difficult problem to determine what is the adequate value of $Q_{NO}/Q_{NO_2}$ for an input. The value of the ratio should be changed according to the mesh size used for calculation. It is not suitable to our mesh size 2 km x 2 km x 100 m, to use the ratio of exhaust gas just emitted from the car. To solve the problem we should make simulation models applicable to smaller scale.

Furthermore, we should pay much attention to the validation of the results. The wind and concentration of pollutants fluctuate in time and space, and emission of pollutants changes with time. Therefore it is difficult to obtain the representative value. Accordingly in validation we should make simulation for a rather long time or for many case-studies. In addition, meteorological model which gives the detailed wind field including diffusivity from the routine observation should be developed, too.

In the present paper, we assumed that the pollutants mixed well in a mesh size and neglected the effects of areosol and any removal process. These are problems to be solved in the future.

**Appendix A**

**Description of scheme MRI-E10**

**A1. Principle**

The basic equation of diffusion eq. (1), given in the text is here rewritten:

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} + V \frac{\partial C}{\partial y} + W \frac{\partial C}{\partial z} = \frac{\partial}{\partial x} \left( K_{H} \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_{H} \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_{H} \frac{\partial C}{\partial z} \right) + Q$$

(A1)

Since the advection terms in eq. (A1) are usually much larger than the diffusion terms, the former should be integrated as accurately as possible. Otherwise we might have trouble with "artificial diffusion".

For this purpose, the horizontal wind is divided into two parts:

$$U(x, y, z, t) = \bar{U}(z, t) + U'(x, y, z, t)$$

$$V(x, y, z, t) = \bar{V}(z, t) + V'(x, y, z, t)$$

where $(\bar{U}, \bar{V})$ are the horizontal wind $(U, V)$ averaged on the $(x, y)$ plane.

Time integration of eq. (A1) is performed by two steps:

In the first step (diffusion stage) we calculate the concentration after the time step $\Delta t$ by the use of the equation:

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} + V \frac{\partial C}{\partial y} + W \frac{\partial C}{\partial z} = \frac{\partial}{\partial x} \left( K_{H} \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_{H} \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_{H} \frac{\partial C}{\partial z} \right) + Q$$

(A2)

In the second step (advection stage) we transport the concentration distribution by the mean horizontal wind $(\bar{U}, \bar{V})$.

**A2. Nomenclature**

In the following finite difference calculation, we apply new notations as:

$$C(x, y, z, t) \rightarrow C_{ijk}$$

$$C(x, y, z, t + \Delta t) \rightarrow C'_{ijk}$$

$$U'(x, y, z, t) \rightarrow U'_{ijk}$$
As seen in the above, \( K_H \) and \( K_s \) are assumed to be functions of height and time only.

**A3. Diffusion stage**

The midway concentration after the time step \( \Delta t \), \( *C_{ijh} \) is given as:

\[
*C_{ijh} = C_{ijh} + \Delta C_{ijh} + Q_{ijh} \Delta t
\]

(A3)

where

\[
\Delta C_{ijh} = \frac{\Delta t}{(\Delta z)^2} [K_H(C_{i+1,j,h} + C_{i-1,j,h} - 2C_{ijh}) + \frac{\Delta t}{(\Delta y)^2} K_H(C_{i,j+1,h} + C_{i,j-1,h} - 2C_{ijh}) + \frac{\Delta t}{(\Delta y)^2} [K_s(C_{ijh - 1} - C_{ijh}) - K_{s,k-1} (C_{ijh} - C_{ijh,k+1})] + \frac{\Delta t}{2\Delta y} U_{ijh}(C_{i+1,j,h} - C_{i-1,j,h}) + \frac{\Delta t}{2\Delta y} V_{ijh}(C_{i,j+1,h} - C_{i,j-1,h}) + \frac{\Delta t}{2\Delta z} W_{ijh}(C_{i,j,h+1} + C_{i,j,h-1})]
\]

(A4)

**A4. Advection stage**

After the diffusion stage, we calculate displacement at the height \( \Delta z \). Displacement in the \( x \) direction \( * \delta_{xh} \) after the time step \( \Delta t \) is given by

\[
* \delta_{xh} = \delta_{xh} + \bar{U}_h \Delta t
\]

(A5)

If \(-\frac{1}{2} \Delta x < * \delta_{xh} \leq \frac{1}{2} \Delta x \), then \( + C_{ijh} = * C_{ijh} \)

and \( + \delta_{xh} = * \delta_{xh} \)

If \( * \delta_{xh} = -\frac{1}{2} \Delta x \), then \( + C_{ijh} = * C_{ijh+1} \)

and \( + \delta_{xh} = * \delta_{xh} + \Delta x \)

If \( * \delta_{xh} \geq \frac{1}{2} \Delta x \), then \( + C_{ijh} = * C_{ijh-1} \)

and \( + \delta_{xh} = * \delta_{xh} - \Delta x \)

Similar procedure is taken for displacement in the \( y \) direction.

**A5. Scheme MRI-E10**

If \( W, \ U/ \bar{U} \) and \( V/ \bar{V} \) are negligible, \( \Delta C_{ijh} \) in eq. (A3) is expressed as:

\[
\Delta C_{ijh} = \frac{\Delta t}{(\Delta z)^2} [K_H(C_{i-1,j,h} + C_{i+1,j,h} + C_{i,j-1,h} + 4C_{ijh}) + \frac{\Delta t}{(\Delta y)^2} [K_s(C_{ijh,k-1} - C_{ijh}) - K_{s,k+1} (C_{ijh,k} - C_{ijh,k+1})]]
\]

Here, we assume \( \Delta x = \Delta y \). We have thus formulated our scheme MRI-E10, and can save the memory and time for computation.

**Appendix B**

**Formulation of chemical reaction model**

Concentrations of \( O_3, NO, NO_2, HC, O, OH, HNO_2 \) and \( RO_2 \) are denoted by \( C_1, C_2 \ldots \) and \( C_8 \) respectively. By the use of Table 1, the rate of formation of species \( i \) \((i = 1, 2, \ldots, 8)\) can be formulated as follows:

\[
RO_2 = \frac{dC_i}{dt} = k_3 C_3 - k_5 C_5 C_4 - k_1 C_1 C_4 \quad (B1)
\]

\[
R_{NO} = \frac{dC_i}{dt} = k_1 C_1 - k_4 C_4 C_6 - k_3 C_3 C_6
\]

(B2)

\[
R_{NO_2} = \frac{dC_i}{dt} = k_1 C_1 + k_2 C_2 + k_3 C_3 C_6 - k_4 C_4 C_8 - k_5 C_5 C_8
\]

(B3)

\[
R_{HC} = \frac{dC_i}{dt} = - k_4 C_4 C_6 - k_5 C_5 C_6 - k_3 C_3 C_6
\]

(B4)

\[
\frac{dC_i}{dt} = - k_4 C_4 C_6 + 0.5 k_6 C_6 C_8 - k_8 C_8 C_8
\]

(B5)

\[
\frac{dC_i}{dt} = k_6 C_6 C_8 + 2 k_7 C_7 C_8 - k_9 C_9 = 0
\]

(B6)

\[
\frac{dC_i}{dt} = -2 k_2 C_2 C_3 + k_3 C_3 C_4 + k_4 C_4 C_5 - k_5 C_5 C_6 - k_6 C_6 C_7 - k_7 C_7 C_8 = 0
\]

(B7)

\[
\frac{dC_i}{dt} = -2 k_2 C_2 C_3 - k_3 C_3 C_4 - k_4 C_4 C_5 - k_5 C_5 C_6 - k_6 C_6 C_7 - k_7 C_7 C_8 = 0
\]

(B8)

Here \( k_j \) \((j = 1, 2, \ldots, 12)\); the reaction number in Table 1 is the rate constant, and we have assumed that \( O, HC, HNO_2 \) and \( RO_2 \) are in a quasi-stationary state; that is, \( dC_i /dt = 0 \) \((i = 5, \ldots, 8)\).

Our procedure for obtaining the concentration is as follows: First, we solve eqs.
(B5), ..., and (B8) for \( C_\alpha \), ..., and \( C_\delta \), assuming that \( C_\mu \), ..., and \( C_\sigma \) are known. By the use of the \( C_\alpha \), ..., and \( C_\delta \) thus obtained and of eqs. (B1), ..., (B4), and (5) in the text, we then calculate the value of \( C_\mu \), ..., and \( C_\sigma \) after the time step \( \Delta t \). And then we reiterate the same procedure.

References


Takeuchi, K., 1976: Recent studies on air pollution model and related meteorological observation in Japan. (submitted to Időjárás, Budapest)


東京地域の光化学スモッグの数値シミュレーション

竹内清秀・木村富士男

東京地域の光化学スモッグの構造を明らかにするため数値シミュレーションを実施した。まず二酸化イオウ \( SO_2 \) と窒素酸化物 \( NO_x \) を不活性気体と見なしして移流拡散のシミュレーションを行い、使用したモデルを評価した後、光化学反応モデルを組入して最終的な光化学反応スモッグの数値シミュレーションを実施した。移流拡散のモデルにはラグランジュ的およびオイラー的の両方の取扱いを試みた。

詳細な気象観測の行われた日の対象にケーススタディを実施した。平均風とともに移動する気塊について考えるラグランジュ的扱いでは、観測的中心の考え方に基づく横方向の拡散を取入れた。光化学反応モデルとして Friedlander and Seinfeld (1969) を用いた。

オイラー的扱いでは、移流拡散に対し「人為的拡散」をふせぐ MRI-E10 スキームを開発し、光化学反応モデルには Eschenroeder and Martinez (1971) および杉山 (1974) を用いた。

一般的にいって、\( SO_2 \) および \( NO_x \) については一応満足すべき結果が得られたと考えられるが、光化学スモッグについてはあまり良い結果は得られなかった。光化学反応シミュレーションの一層の開発が望まれる。