10.4 The Practical Method of Estimating Air Pollution

How is the diffusion simulation model which was described above used in the estimation of actual atmospheric environment? Also, what kind of data are gathered, analyzed and used? Here, an example is given of the forecasting model with an actual atmospheric environment concentration.

10.4.1 Estimating the long-term concentration

The type of concentration that can be most accurately diffusion by the present air pollution forecasting model is the long-term average such as the annual average or the seasonal average concentration. The primary reason for this is, the fact that the diffusion phenomenon is basically a statistical phenomenon and the ability to estimate the concentration at a point and time is only statistical. However, the long-range averages like the annual average or the seasonal average are made up of the average of the collections of many one-hour averages. Thus, the statistical uncertainty decreases. Other error factors are the errors in the field of diffusion and estimation errors at the emission source.

At present, the long-term average density estimate which uses analytical solution models such as the plume and puff models is regularly used for the above reason and is used to estimate the concentration of sulfur oxides and nitrogen oxides. The emission source, the weather and the environment concentration data are all necessary to estimate the long-range average concentration. The flow chart of the simulation of long-term average for the total emission control method of sulfur oxides and nitrogen oxides in Japan is conducted with the procedures in Fig. 10.4.1.

For example, from the data on the solar radiation and the wind direction and velocity for every hour of 365 days or one year, the occurrence frequency of the meteorological condition is calculated for the stability of the atmosphere and for the class of wind velocity of each of the sixteen directions.

The sorting of the wind velocity class and the stability of the atmosphere is due to the Japan standard stability classification as shown in Table 10.4.1. This classification list is an improved version of the one which was proposed by Pasquil of the UK. Pasquil's method displayed the strength of the solar radiation with the cloud volume, but, in the Japan standard stability classification, Pasquil's method has been changed into solar radiation which is a quantitative indicator. This method evaluates the convection and the strength of the inversion layer by the surface wind velocity and the solar radiation or the net radiation, and classifies stability. As for stability, A-C are unstable, D is neutral and E and F are stable. Pasquil and Gifford gave plume width to each stability as seen in the graphs in Fig. 10.4.2.

The annual average concentration uses the data of pollutant emission which was estimated according to the time zone and season, and is computed using the wind direction, the wind velocity and the occurrence frequency of thermal stability of the atmosphere which were ordered according to the time zone and season. To estimate the pollutant emission in this case, the emission coefficient which was introduced in Chapter 6 section 8 is utilized.
Fig. 10.4.1 The estimated flow of the long-term average concentration

<table>
<thead>
<tr>
<th>Ground level</th>
<th>Daytime Solar radiation amount</th>
<th>Thick night cloud</th>
<th>Nighttime</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wind velocity (m/sec)</td>
<td>&gt;50</td>
<td>49~25</td>
<td>&lt;24</td>
</tr>
<tr>
<td>&lt;2</td>
<td>A</td>
<td>A~B</td>
<td>B</td>
</tr>
<tr>
<td>2~3</td>
<td>A~B</td>
<td>B</td>
<td>C</td>
</tr>
<tr>
<td>3~4</td>
<td>B</td>
<td>B~C</td>
<td>C</td>
</tr>
<tr>
<td>4~6</td>
<td>C</td>
<td>C~D</td>
<td>D</td>
</tr>
<tr>
<td>&gt;6</td>
<td>C</td>
<td>D</td>
<td>D</td>
</tr>
</tbody>
</table>

Note: The numerical value considered Japan’s climate for the solar radiation ranking of Pasquil’s stability classification table.
Fig. 10.4.2 Plume width for the atmospheric stability by Pasquill's method

Fig. 10.4.3 Scatter diagram showing the computation value and the measurement value of SO₂ annual average from the puff and plume models.

Fig. 10.4.3 scatter diagram comparing the measurement value (horizontal) and the calculated value (vertical) computed by using the above method of simulation. If the point is located on the 45 degree line, the calculation value and the measurement value agree totally. However, the computational value becomes lower than the measurement value because there are unknown sources which is not able to cover is the simulation. and, also, because
the pollutant is transported from an outside area. This difference is called background concentration. If the computational value is $x$, the measurement value is $y$, and the background is $b$ then the relationship between the measured and the computational value is approximated using Eq. (17).

$$y = ax + b$$

(17)

Here, $a$ is a proportional coefficient with the measurement value and the computation value.

The agreement of the simulation is evaluated by the correlation coefficient with the measurement value and the computation value along with coefficient $a$. The simulation becomes highly precise when the correlation coefficient is near 1 and $a$ is near 1 in the calculation. A case of a non-heating period is shown in Fig. 10.4.4 as an example of the diffusion calculation results with an seasonal average concentration in the area.

![Annual average concentration profile from the puff and plume models](image)

Fig. 10.4.4 A long-term average concentration profile from the puff and plume models

A personal computer program, which estimates the long-term average concentration of the plume and puff models is sold. A program which statistically analyzes the meteorological condition from the weather data such as the wind direction, wind velocity, and solar radiation is also available.
10.4.2 Estimating the short-term average concentration

The numerical simulation models, described in section 2, are used for the estimation of the concentration under specific meteorological conditions and of the diffusion under complex topography along with the plume and puff models. A numerical simulation model is used often for the diffusion calculation for sea-land breeze condition. Shown in Fig. 10.4.5 is a computation example of a simulation of the sea-land breeze on the Kanto Plain using the numerical simulation model. This displays the vector of the wind direction and the wind velocity near ground level. This numerical model is considering the latent heat flux and a sensible heat flux produced between the ground surface and the atmosphere by the solar radiation.

It becomes possible with the plume and puff models to estimate the short-term diffusion concentration in an actual situation by introducing the wind direction and velocity and, also, the change in the height of the plume width, etc. In addition, the box model, the limited length plume model and the floating puff model are used for diffusion calculation when there is a change in the field of diffusion during the time. Shown in Fig. 10.4.6 is the concept figure of a floating puff model and a limited length plume model.

Fig. 10.4.5 Distribution of surface winds on the Kanto Plain in the case of sea-land breeze from a numerical simulation model
10.4.3 Estimating chemically reactive substances

The environmental concentration simulation of the material which reacts chemically in the atmosphere, the process of the chemical change should be simulated along with the diffusion process. The photochemical reaction is involved in the chemical change in most cases. The representative reactions are oxidants generated through photochemical reactions, nitrogen oxides formed into nitrogen dioxide, sulfates and acid substances formed from sulfur dioxide, particulate matter formed from nitrogen oxides and hydrocarbon species and destruction of the ozone in the stratosphere.

Several tens of chemical substances and twice or more that of the reaction formulas are considered in the simulation of photochemical oxidants. The representative chemical substances are non-methane hydrocarbon, nitrogen oxides etc. The non-methane hydrocarbon is classified into ethylene, aromatic and aliphatic hydrocarbons, excluding ethylene and a carbonyl compound excluding formaldehyde.

Regarding the reaction of nitrogen oxides (NO→NO₂), in the case like the diffusion of a short distance, the reaction of NO and O₂ is the quickest reaction and the photochemical reaction can be disregarded. Then, NO, NO₂, O₁ O₂ and the intensity of ultraviolet radiation are applied. A reaction formula is shown in Eq. (18) but the details of the reaction have been described in Chapter 4 section 2.

\[
\begin{align*}
\text{NO} + \text{O}_2 & \rightarrow \text{NO}_2 + \text{O}_2 \\
\text{NO}_2 + h \nu & \rightarrow \text{NO} + \text{O} \\
\text{O} + \text{O}_2 & \rightarrow \text{O}_3
\end{align*}
\]
For the total emission control for nitrogen oxides in Japan, the method (exponential function model) of Eq. (19) which simplified this reaction system is used.

\[
\frac{\text{NO}_y}{\text{NOx}} = 1 - \frac{\alpha}{1 + \beta} \left\{ \exp (-k t) + \beta \right\} \tag{19}
\]

Here, \(\alpha\) is the rate of NO at the emission source, \(\beta\) is the numerical value related to the rate of NO when its reaction reaches an equilibrium, and \(k\) is a reactive constant. Also, the value of these coefficients are as follows:

\[
k = 0.0062 \ \text{UO}_\text{in} \ \text{(stationary sources, vessels)}
\]

\[
= 0.208 \ \text{UO}_\text{in} \ \text{(automobiles, houses)}
\]

\[
\beta = 0.3
\]

\[
\alpha = 0.9
\]

Here, \(U\) is velocity and \(O\_\text{in}\) is concentration of Ozone.

Other than the method above, there is another method using Eq. (20) (statistical model) in which the ratio is statistically processed from the observed data of nitrogen oxides.

\[
\text{NO}_y = a \left\{ \text{NOx} \right\} b \tag{20}
\]

Here, the coefficients \(a\) and \(b\) are determined through the analysis of observed data.

In the estimate of environment concentration, an exponential function model is used when the contribution of each stationary source are required and the statistical model is used when computing the influence of automobiles.

10.4.4 Estimating from wind tunnel tests

Wind tunnel tests are utilized in conjunction with numerical models in the simulation of diffusion when the so-called down-washes and down-drafts, affect the diffusion due to topography or buildings, for example, effects from the wake in the lee of buildings and smoke stacks. An example of wind tunnel equipment is shown in Fig. 10.4.7.
The wind tunnel consists of a blower, a flow control section, a test section and a re-circulation section. In the diffusion wind tunnel test, instead of smoke, a tracer gas flows from the model stack over a model topography or building which was built in the test section, then tracer gas is sampled in the downstream side and analyzed. To make it similar to the turbulent boundary layer of the atmosphere, a turbulence generator and a roughness element are placed in the upstream side of the test section. To develop a sufficient turbulent flow boundary layer, an approach distance of at least 2 to 5 meters is necessary and a test section length of more than 5 meters is required. Scale model of 1/100 to 1/1,000 in the case of buildings and for topographic model the scale of 1 to several hundredths to 1 to several thousandths is used.

As a tracer gas for the diffusion experiment, a kind of hydrocarbon such as ethylene or propane is used. The wind velocity in the wind tunnel test is the same or a little less than the actual velocity. Therefore, the range of the wind velocity which is required for the diffusion wind tunnel is approximately 1 to 10 m/s. Photo. 10.4.1 shows the diffusion of smoke in a wind tunnel test.
Photo 10.4.1  Smoke diffusion experiment with a diffusion wind tunnel