A NUMERICAL SIMULATION OF SECONDARY SPM ORIGINATED FROM AUTOMOBILES WITH LAGRANGIAN MODEL

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1. Introduction

A variety of numerical simulation models of air pollution have been developed in recent years. The Eulerian models are suitable for simulating relatively larger-scale pollution, but unsuitable for simulating smaller-scale phenomena caused by a specified point source. When environmental effects of a specified road construction is assessed, enormous calculation capacity is required to cover a wide range of spatial scale from a road size or building size to urban or mesoscale even if the nesting grid method is used to reduce a calculation load.

In contrast, Lagrangian models are suitable for simulating small spatial and time scale phenomena because the model can avoid the obstructive numerical diffusion. The Lagrangian models have never been applied for simulation of pollution with photochemical reactions partly because no interaction among Lagrangian particles can be considered. Nevertheless if a pollution simulation which cover a wide range of spatial and time scales can be divided into the Eulerian and the Lagrangian models according to their strong and weak points, large amount of calculation resources will be reduced.

In this study, a Lagrangian model that can simulate behavior of the secondary particles of SPM is developed. The model is equipped with an ordinary photochemical reaction sub-model and a sub-model for a series of chemical reaction process of the secondary particles of SPM from generation to deposition. Each Lagrangian particle has the same functions as the box model [1, 2] and the puff. Trajectory of the particle is calculated by a similar manner to the Monte Carlo Simulation. The model is applied to SPM pollution events caused by automobiles in Osaka Prefecture, Japan. The validity of the model is checked by comparing with observed data.

2. SPM simulation model

2.1 Sub-model for convection and diffusion calculations

Convection and diffusion of pollutants are calculated by the RAPTAD (Random Puff Transport and Diffusion). All the pollutants including secondary particles of SPM are assumed to be contained by puffs. The Puff is transported by wind that include random component generated by turbulence. Diffusion width of the puff is expanded with convection. A series of pollution process including photochemical reactions, generation and deposition of pollutants are assumed to occur only inside puffs. Each of the puffs is regarded as a box model. Concentration of a pollutant at a grid point is calculated by linearly summing the pollutant concentrations derived from each puff over all the puffs existing in the calculation domain. Any interactions among the puffs are neglected.

Distribution of a pollutant concentration in a puff is assumed be the Gaussian distribution as follows;

$$c_k(x,y,z)=\frac{m_k}{(2\pi)^{3/2}\sigma_{xk}\sigma_{yk}\sigma_{zk}}\exp\left\{-\frac{1}{2}\left(\frac{(X_k-x)^2}{\sigma_{xk}{}^2}+\frac{(Y_k-y)^2}{\sigma_{yk}{}^2}+\frac{(Z_k-z)^2}{\sigma_{zk}{}^2}\right)\right\} \quad (2\text{-}1)$$

where $c_k(x,y,z)$ is concentration derived from the kth puff at a (x,y,z) point; m_k is mass of pollutant included by the kth puff; Δt is time interval of puff generation; σ_{xk} is diffusion width of the kth puff in x-direction that is a standard deviation of Gaussian distribution; (X_k, Y_k, Z_k) is a position of the center of the kth puff. The initial diffusion width in the vertical direction and the initial height of the puff center above the ground level are fixed to 100m and 10m, respectively. The interval of puff generations is set to be 3600s.

2.2 Sub-models of photochemical reaction and generation of secondary particles of SPM

The CBM-IV [3] that is the most prevailing model of the carbon-bond approach is used as the sub-model for simulation of photochemical reactions in this study. Some models to simulate generation of secondary particle of SPM such as the Japan Environment Agency Model (the JEA model), the De More model and the Equilibrium Model have been developed. [2] According to the JEA Model [4], interchange of a gaseous pollutant and SPM is calculated using following equations:

$$\frac{d[GAS]}{dt}=-P_k k_t[GAS]+(1-P_k)\frac{k_t}{A}[SPM] \quad (2\text{-}2)$$

$$\frac{d[SPM]}{dt}=P_k A k_t[GAS]-(1-P_k)k_t[SPM] \quad (2\text{-}3)$$

where $[GAS](ppb)$ is concentration of gaseous matter, $[SPM](\mu g/m^3)$ is concentration of SPM, $A\,(\mu g/m^3/ppb)$ is a coefficient of transformation of gas into SPM, $k_t\,(1/h)$ is reaction rate that gas transforms to SPM, and P_k is proportion of SPM to all form of pollutant. The above equations are applied to transformation of NOx into nitrate and SOx into sulfate. NO2 and SO2 are assumed to be precursors of nitrate and sulfate respectively. According to JEA [4] and Harada [2], coefficients are set as listed in Table 2-1. Reaction rate of SOx to all forms of SPM is assumed to be 1.

The model covers only fine weather days therefore the effects of wet deposition are neglected. The treatment of dry deposition is the same as that in the manual compiled by the JEA. The effect of dry deposition is represented by mass reductions of gaseous pollutants or SPM included in puffs. The reduction of a pollutant mass Δm is defined as follows:

$$\Delta m / m = V_d \Delta t / \sigma_{zk} \quad (2\text{-}4)$$

where m (g) is total mass of a pollutant contained by a puff, V_d (m/s) is a dry deposition velocity which is listed in Table 2-2, Δt (s) is a time step, σ_{zk} (m) is a diffusion width in the vertical direction. The equation means that ratio of the mass reduction of a pollutant to its total mass contained by a puff is equal to ratio of a settling distance of the pollutant to the diffusion width of the puff.

Table 2-1 Parameters in JEA model

	Variable	Summe	Winter
A_S	Transformation coefficient of SO_X into SO_4^{2-}	4.29	
A_N	Transformation coefficient of NO_X into NO_3^{-}	2.76	
K_{tS}	Reaction rate of SO_X to SO_4^{2-}	0.05	0.04
K_{tN}	Reaction rate of NO_X to NO_3^{-}	0.065	0.05
P_{kN}	Proportion of SPM to NO_X	0.6	0.8

Table 2-2 Dry deposition velocity

Species	$V_d\,(m/s)$
NO	0.001
NO_2	0.001
O_3	0.006
SO_2	0.008
HC	0.002
HNO_3	0.002
SPM	0.001

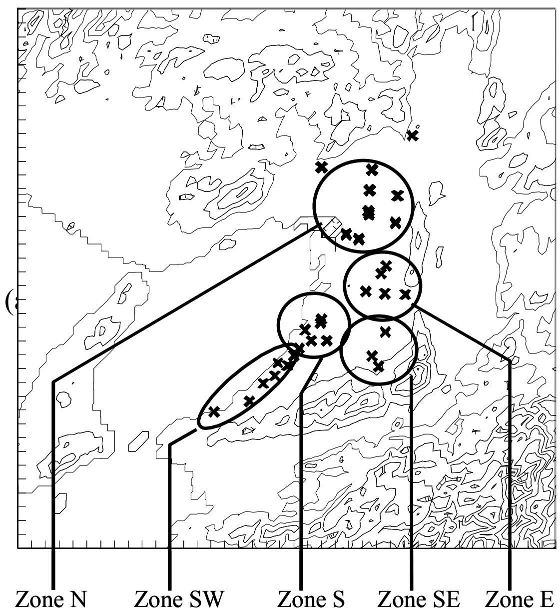
2.3 Model for simulation of wind field

The HOTMAC (Higher Order Turbulence Model for Atmospheric Circulation) [5] is used to calculate atmospheric circulation. The upper-air observation data by the Japan Meteorological Agency is used to introduce effects of the wind field, of which scale is larger than the model can predict, into the simulation by the nudging method. The velocity vectors obtained at the level of 850 hPa every 6hr were introduced into calculation grids 1500m and higher above the sea level. Wind vector data near the ground surface by the Automated Meteorological Data Acquisition System (AMeDAS) is also introduced to relax the calculated state toward the observed state.

3. Observation data of SPM

Air pollution data which the Osaka Prefecture Government collects at twenty-eight points shown in Fig 3-1 were used to examine the validity of the model. Pollutants concentrations are easily affected by conditions of local areas around observation stations. The mesh size of the model is too coarse to simulate pollution phenomena within the local area. Therefore the observation data is divided into five groups according to their geographic positions to get spatially averaged values. The averaged data of each group are compared to the calculated results.

Fig.3-2 depicts time series of the averaged concentration of SPM. Fluctuations of the averaged concentrations in the Case 2 were at a lower level and relatively flat because the clear air wind caused by the pressure gradient blows the pollutants off the calculation domain. Because of the mild spatial gradient of atmospheric pressure, sea and land breeze was likely to occur in the Case 1. In the Case 1, variation of about 24hr period can be seen in the averaged concentration for all the zones. The periodical variation is mainly caused by that the land and sea beeze, emission of pollutants and photochemical reactions have a period of 24hr.



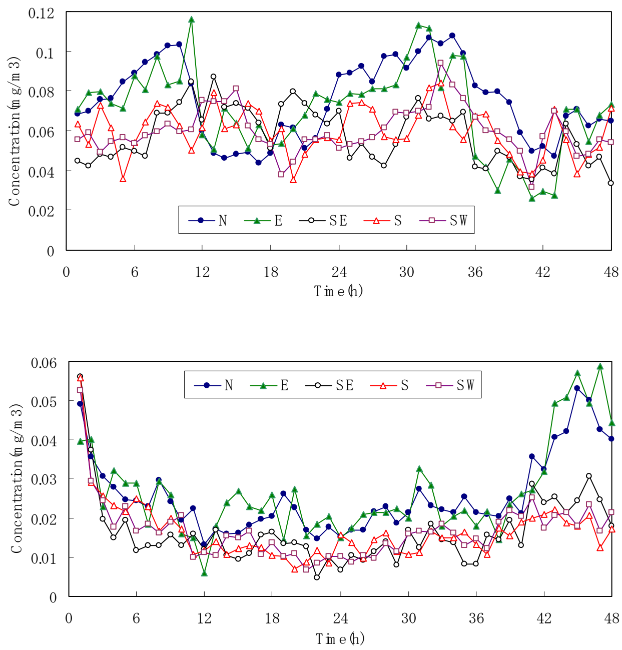


Fig3-1 Observation Station of air pollution in Osaka Prefecture

(b) Case 2

Fig3-2 Observation data of SPM

4. Calculation method

4.1 Calculation domain and condition

The calculation domain is depicted in the Fig.4-1. The domain covers the Osaka Prefecture area and a part of the Osaka Bay. The origin (the south-west corner) of the calculation domain is lat. 34.07N and long. 134.73E; the domain sizes in latitudinal, longitudinal and vertical directions are 117km, 117km and 5km respectively. The horizontal grid size is 3km. 15 variable-sized grids cover the calculation domain. Variation of SPM concentration is closely related to meteorological features of wind fields. So here we selected two typical weather conditions listed in the Table 4-1.

Table 4-1 Calculation condition

Case	Outlines of weather condition	Date
I	Fine weather. Pressure gradient of large scale is small. Land and sea breeze clearly occurred.	18 Aug. 1995
II	Fine weather. Wind caused by large scale pressure gradient dominates. No land and sea breeze was observed.	1 Nov. 1995

4.2 Estimation of pollutants emission

Emission rates of pollutants by automobiles are estimated road by road using the traffic census data for 1990 [6]. Considering that the model can't simulate pollution phenomena of which scale is less than the mesh size, innumerable road to road emission data are aggregated into emission data by municipality. Each of the 44 circles in Fig 4-1 corresponds to a municipality in the Osaka Pref.; the circle center and the circle area represent a position of the government office and the municipal area, respectively. Puffs containing automobile pollutants by municipality randomly occur within each of the circles. Fig.4-2 shows time series of NOx emission rate for some municipalities.

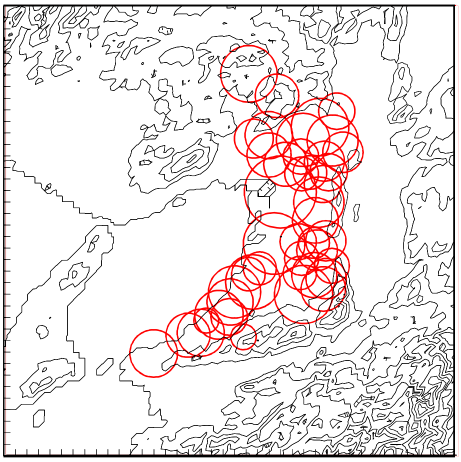


Fig 4-1 Circles expressing municipalities

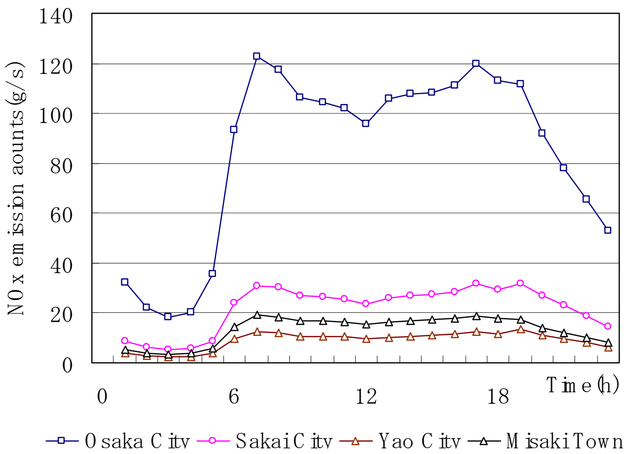


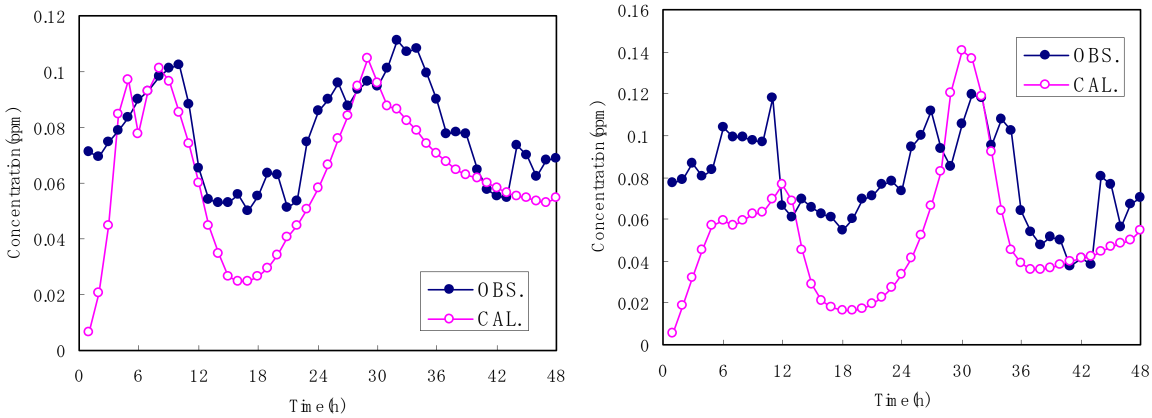
Fig 4-2 Time series of NOx emission

5. Results

Fig 5-1 and 5-2 show comparisons between calculated and observed concentrations of SPM in the Case1 and the Case2. The calculated concentration contains only the secondary particle of SPM and the observed one covers both the primary and the secondary particles of SPM. However because ratio of the primary SPM to the total SPM is usually only 10 to 30% in the calculated domain, the comparison is thought to be meaningful. Difference in hourly variations of the zonal concentration between the two cases is expressed by the model simulation quite well. In the Case1, the model adequately predicts that only one concentration peak occurs in the morning commuter time in a day although there are two peaks in variation of the emission rate. This is cased by that turbulence diffusion is suppressed by inversion layer which develops in the night time. The levels of calculated concentration are lower than those of observed one on the whole, because the simulation does not calculate any emission sources but the automobiles.

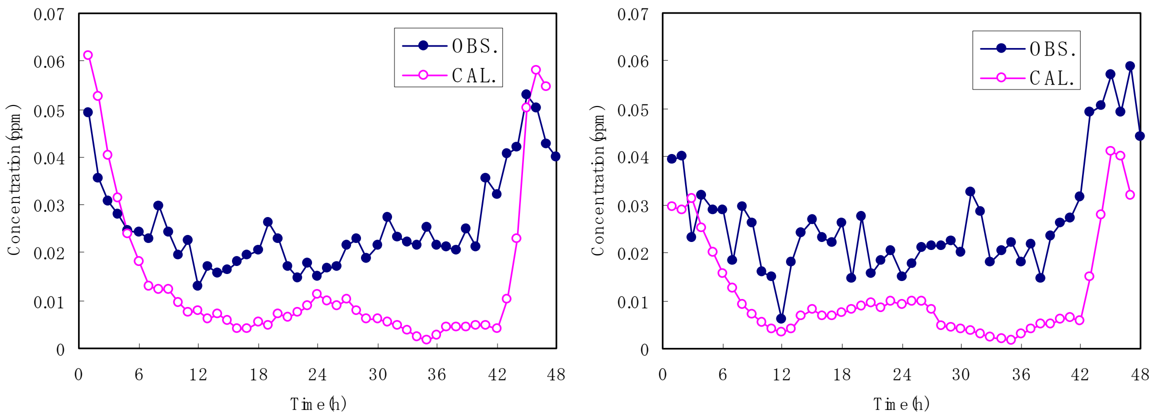
6. Conclusions

The Lagrangian simulation model combined with the photochemical reaction model and the generation model of secondary particle of SPM has been proposed. Simulation of the SPM pollution events by automobiles in the Osaka Prefecture area was carried out. Even though the model calculated only the secondary particle of SPM originated from automobiles and it treated pollutants emission as non-point source for each municipality, the model predicted the differences in temporal variation of SPM concentration due to weather conditions quite well. Validity of the model will be examined by taking account of many other sources of pollutants as well as primary particle of SPM.



(a) Zone N (b) Zone E

Fig 5-1 Time series of SPM concentration (Case 1)



(a) Zone N (b) Zone E

Fig 5-2 Time series of SPM concentration (Case 2)

References

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