A Consideration on Air Quality Models for Environmental Assessment*

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Air quality models are used for many aspects of environmental management ; environmental assessment and so on. Recently, the quality assurance for softwear goods became an important concern. The air quality model can not be an exception. The air quality models for regulatory use should have a good predictive performance. This performance is usually measured by statistical scores, and varied depending on the regulatory purposes.

INTRODUCTION

In order to carry out an environmental implementation planning or to make a strategy for environmental management, tools for predicting environmental quality are necessary and the quality of the tools become an important concern. Air quality models are used for many kinds of environmental decision-making. For many countries, the use of these air quality models has become an unavoidable requirement for determining acceptable emission levels so as not to excess the atmospheric environmental standards.

The air quality models are sometimes devided into two groups: one is a model for regulatory use, the other is a model for research. The regulatory models should not be only the convenient models for officers, but should also be the models which have sufficient predictive performance for regulations. The regulatory models require higher levels of the appropriateness and usefulness than the research models do.

This article describes the fundamental components of the air quality models for regulatory use.

LONG-TERM MODELS VS SHORT-TERM MODELS

The averaging time of concentrations predicted by air quality models should be consistent with the environmental standard or any regulatory goals. The sulfur dioxide national ambient air quality standards (NAAQS) in U.S. and Japan are shown in Table 1. Since the NAAQS for each country is not the same, there should be some difference in the air quality models depending on the countries.

The urban air quality model of the initial

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Table 1 SO_2 national ambient air quality standards (NAAQS) in U.S. and Japan

U.S.	primary NAAQS		
		80 μg/m³ (0.03ppm)	—Annual arithmetic mean
		365 μg/m³ (0.14ppm)	—Maximum 24-hr conc. not to be exceeded more than once per year (second highest value)
	secondary NAAQS		
		1300 μg/m³ (0.50ppm)	—Maximum 3-hr conc. not to be exceeded more than once per year (second highest value)
Japan	(i) 0.04 ppm		—Maximum 24-hr conc. not to be exceeded more than 2% per year (98-th percentile value)
	(ii) 0.10 ppm		—Maximum 1-hr conc. not to be exceeded
	cf : warning condition		
		(i) 0.5 ppm	3-hr conc. exceed this value
		(ii) 0.7 ppm	2-hr conc. exceed this value

stage was developed for predicting the annual average concentrations. Examples of these categories are AQDM and CDM of the United States. Almost all of the regulatory models used in Japan belong to this type, namely long-term models for the prediction of annual average concentrations.

The averaging times for many kinds of air pollutants in NAAQS are not the annual average, but the average for several hours or the daily average. The famous statistical analysis proposed by Larsen (1969) assists the use of long-term models for these pollutants. The essence of Larsen's theory is that there exist the interrelations between the percentile concentrations (for example, 98%-value) and the averaging time, and any desired averaging-time concentrations can be estimated from the other averaging-time concentrations. Therefore, 98%-value is estimated from the annual average concentration which is predicted by a long-term diffusion model.

However, recently this theory was found to be applicable only in the urban area. In the guideline for air quality models of U.S.EPA, it is recommended that the Larsen's theory should not be used for an isolated source or an emission source in complex situations. On the basis of the knowledge described above, U.S.EPA proposed the CRSTER, MPTER and many other models for the environmental assessment. This kind of models belong to the short-term models, and are able to predict the hourly maximum concentrations directly.

APPLICATION OF AIR QUALITY MODELS

The air quality models are used for predicting the pollution levels of various kinds of temporal scale and spatial scale. The smallest scale may be indoor pollution by radon or cigarette smoke and so on. The

Table 2 Statistical evaluation scores for the Total Pollution Load Control (Implementation planning program in Japan)

(i) regression coefficient b (obs. = a + b * cal.)	$0.8 \leqq b \leqq 1.2$ (desirable)
(ii) correlation coefficient r	$r \geqq 0.71$ (necessary) $r \geqq 0.8$ (desirable)
(iii) spatial distribution	Concentration field obtained by AQM should be consistent with observed one.
※ Additional conditions for NO_2 AQM	
(iv) bias a_0 ($a_0 = \overline{obs.} - \overline{cal.}$)	$a_0 \leqq 1/3$ (obs.-BG)+BG where BG is natural background conc.
(v) residual variance s'^2 $s'^2 = 1/(n-2) \cdot \Sigma(obs.-cal.-a_0)^2$	s'/obs.< 1/4
(vi) s'	s'/obs.< 1/5
For NO_2 AQM, (i)(ii)(iv)(v) or (iv)(vi) should be attaind.	

All values in this table are annual average concentrations.

largest scale is a global scale air pollution caused by CFCs and secondary acid aerosols, etc.

Temporal scale of the air quality models are also important factors. For the environmental risk assessment concerning the facilities of highly flammable or explosive materials, it is quite useless to predict its hourly average concentration. In case of the assessment for dangerous chemicals, less than a few seconds average values should be calculated.

The aim of air quality simulation can be classified by the regulatory use. The other factors of importance for air quality simulation are the state of the location: already polluted aera where the implementation planning should be applied, or the relatively clean area where a new emission source will be constructed. Examples for the former case are the U.S. state implementation planning (SIP) or Total Pollution Load Control (TPLC) in Japan. The most important applications for the latter case may be the environmental assessment.

AIR QUALITY MODELS FOR THE TOTAL POLLUTION LAOD CONTROL IN JAPAN

Total pollution load control (TPLC) in Japan is nearly equivalent to State Implementation Planning in the United States. Its role is to attain the air quality standard by implementating the preventive measures. In order to carry out the TPLC, the relationship between the ambient concentration and emission should be explained by sound and scientific means. An air quality model based on the Gaussian plume diffusion equation is generally used for this purpose. This model is very similar to CDM and AQDM in the United States. The greatest difference of the Japanese system from the U.S. system consist in that simulations are carried out based on the data of past reference years in advance of the prediction and that the calculated and measured va-

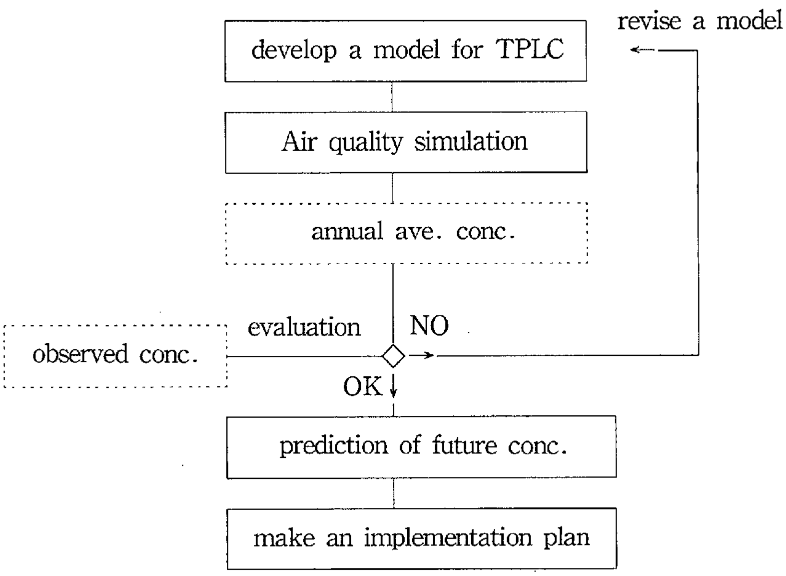

Figure 1 Schematic diagram for Total Pollution Load Control (TPLC).

lues must be consistent with each other in reasonable accuracy. The evaluation standards for the validation are shown in Table 2. If model performance is not sufficient, not only the emission inventory must be reviewed, but the diffusion model and diffusion parameters must also be reexamined (See Figure 1). Strict specifications as in "Guideline on Air Quality Models" in the U.S. are therefore not set for the diffusion models in TPLC in Japan. This system is supported by the largest air quality monitoring network in the world : it consists of more than 1600 stations throughout Japan and the monitoring stations are located in most of the urban and industrial areas.

The TPLC for sulfur dioxide in Japan was carried out satisfactorily, and in most cases sufficient results could be attained to a certain extent by using models for predicting annual average values only. However, if a pollution source with a high contribution rate to the average annual value and a source with a particularly high contribution rate to the high concentration (episodic condition)differ when environmental standards cannot be attained because of high concentration pollution occurring several times, despite the fact that the annual average value is not very high, assurance of attaining environmental standards will be difficult even if the contribution rate of each emission source to the annual average value is calculated with the air quality model and preventive measures for the source based on these calculated values are proposed (Shiozawa, et al., 1990).

The air quality model used in the TPLC for nitrogen dioxide in Japan is similar to that for sulfur dioxide. The TPLC for NOx was not successful. One of the possible reasons for this failure of the attainment of the nitrogen dioxide air quality standard(NO_2 AQS) may be that, although NO_2 AQS are set for the 98th percentile value of daily average concentration, the target values are usually set for the annual average values equivalent to the daily average 98th percentile value, and the implementations towards this target value was carried out. In most cases, the annual average value equivalent to daily average 98th percentile value of 0.06ppm (NO_2 AQS) is estimated by statistical methods such as regression analysis. This target value is generally about 0.03ppm.

However, Kannari et al.(1989) have pointed out that variations in the annual average value equivalent to the daily average 98th percentile value are large depending on the year. According to this report, analysing annual data for the 10 years period from 1978 to 1987 in the Tokyo metropolitan area, the annual average value corresponding to the above mentioned 0.06ppm of daily average 98th percentile value is within the range of 0.025 to 0.035ppm.

It is also necessary to consider the problem on the confidence limit of regression analysis. Figure 2 shows the results of the regression analysis conducted on data of the monitoring stations in Tokyo metropolitan area. The 95% confidence limit for the regression line and the individual data points are also shown in this scatter diagram. It is inferred that the annual average target value will be about 0.02 to 0.025ppm in case that 98th percentile value of daily average concentration must be

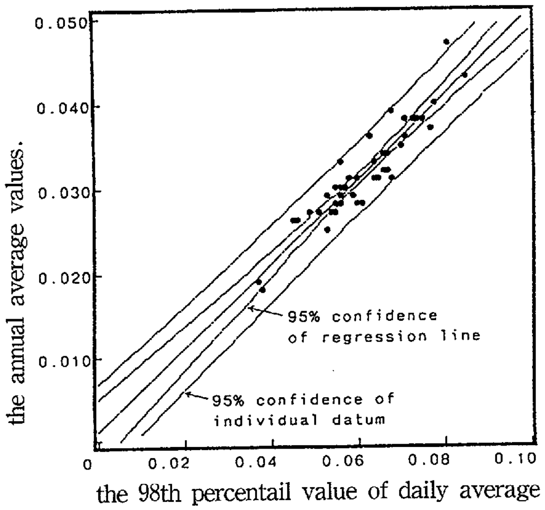

Figure 2 Regression analysis for the target values of annual average concentrations equivalent to daily average 98% values. (April 1991 - March 1992, Tokyo area)

less than 0.06ppm with the estimated uncertainty based on the regression analysis.

AIR QUALITY MODELS - COMPARISON WITH U.S. MODELS

The air quality models used in Japanese total pollution load control belong to the most famous models in Japan. In this Japanese models, a great deal of matters are left to user's discretion. As long as the validation process of the air quality model is carried out, this discretion effectively fulfills its function. Since in Japan almost all urban areas have more than several air monitoring stations, this system is better than the U.S. system in which the discretionary change to the regulatory model is prohibited. Since much of the U.S. models are released as the form of computer source list, we can easily modify and refine these models. But these modified models are no longer considered as the U.S.EPA's approved model.

Concerning the air quality models used for an environmental assessment, this situation is quite different. The validation process of air quality models is usually skipped. If the air quality models for an environmental assessment have the same discretion as those for the total pollution load control and the validation is not carried out, any desired values for the predicted concentration can be obtained by this air quality model at the discretion of the users.

U.S.EPA presented the guideline on air quality models and revised it in 1993 (U.S. EPA, 1993). This revised guideline shows the recommended air quality models for regulatory applications (see Table 3). These models are specified by standard FORTRAN source listing along with the user's manual(s). The basic requirements for the U.S.EPA's recommended air quality models are presented in U.S. Federal Register (45FR20157). One of these requirements is to be evaluated by a sufficient size of data or authorized predictive tools. The aim of this system is not to make an excellent model for the typical area with many air monitoring stations, but to develop a model with minimal predictive performance even if this model is applied to the area with no air monitoring stations.

Another important difference between U.S. models for environmental assessment and Japanese models is the objective concerning the concentrations predicted. The types of air quality simulation may be devided into five groups as shown in Table 4. Some people believe that a short-term model should

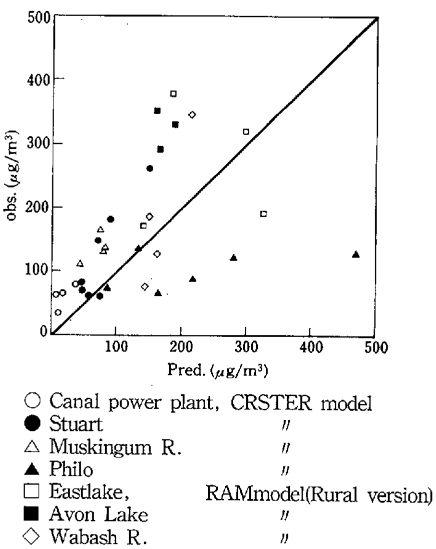

Figure 3 Scatter diagram for second highest values of daily average SO_2 concentrations during about one year. The predicted values were obtained by RAM (Ellis & Liu, 1981) and CRSTER (Lee et al., 1975) models.

Table 3 Recommended air quality models (AQM) in U.S. EPA's revised guideline

level of recommendation	name of air quality simulation model
Preferred AQM	BLP : Buoyant line and point source dispersion model
	CALINE 3 : (California line source model)
	CDM 2.0 : Climatological dispersion model
	RAM : Gaussian-plume multiple source air quality algorithm
	ISC2 : Industrial source complex model
	MPTER : Multiple point Gaussian dispersion algorithm with terrain adjustment
	CRSTER : Single source model
	UAM : Urban airshed model
	OCD : Offshore and coastal dispersion model
	EDMS : Emissions and dispersion model system
	CTDMPLUS : Complex terrain dispersion model plus algorithms for unstable situations
Alternative AQM	AQDM, ARRPA, APRAC-3, COMPTER, ERT-Visibility model, HIWAY-2, IMPACT, LONGZ, PPSP, MESOPUFF-II, MTDDIS, models 3141 and 4141, MULTIMAX, SCSTER, PG&E plumes model, PLMSTAR, PLUVUE-II, PAL-DS, RADM, RPM-II, RTM-II, SHORTZ, GMLINE, TCM-2, TEM-8, AVACTA-II, SDM, WYND valley model, DEGADIS

Table 4 Type of the Air Quality Simulation

No.	Type	Application
1	– Maximum (or second highest) concentration at anyplace and anytime during the designated period (usually one year)	PSD, NSR etc.
2	– Maximum (or second highest) concentration at designated place and at anytime within the given duration (one year)	PSD, NSR etc.
3	– Maximum or representative concentration at anyplace and at the designated time	O_3 control in AQMP etc.
4	– Concentration at the designated place and time	Real-time emission control etc.
5	– Probability distribution or long-team average values of the concentrations at anyplace or at designated place during the given period (one year)	SIP, AQMP, EIS etc.

PSD: Prevention of significant Deterioration, NSR: New source review
SIP: State implementation planning EIS: Environmental impact statement
AQMP: Air quality maintenance planning

predict the concentrations at the designated place and time (type 4). This type of simulation is the most difficult one, and sometimes it may be required, for example, for photochemical air pollution prevention. However, most of the U.S. short-term models such as CRSTER and MPTER are made towards the aim of type 1: to obtain the maximum (or second highest) concentrations at anyplace and anytime during the designated duration (usually one year).

Most of the Japanese also believe that any diffusion models cannot predict the highest concentrations. This belief is correct when only a Japanese air quality model for total pollution load control is used, because many parameters such as diffusion coefficients are used for the prediction of long-term average concentrations. This belief is not valid in case of CRSTER or similar models. Some evidence is shown in Figure 3. Although there is a deal of scatters of the data, this scatter diagram does not show a systematic bias. The reason for this tendency is that many parameters including diffusion coefficients are consistent with the aim of type 1 simulations. However, since many Japanese models are made for prediction of annual average and not towords the aim of type 1, the predictive performance for the highest values may be poor (see Figure 4). This tendency is reversal for the prediction of long-term average values or nearly 50th percentile concentrations. It is obvious from EPA model evaluation study that CRSTER and similar models can not predict the long-term average and less than 90th percentile concentrations with sufficient accuracy, and the predictive performance of these U.S. models for nearly 50 to 70 percentile values may be inferior to the Japanese system.

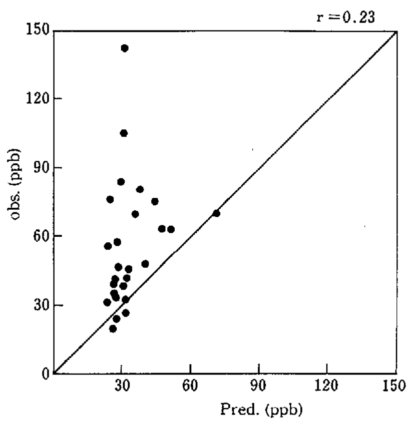

Figure 4 Scatter diagram for second highest values of one-hour SO_2 concentrations during one year (April 1980 - March 1981, Kashima area). The predicted values were obtained by the long-term model for TPLC.

QUALITY ASSURANCE FOR AIR QUALITY MODELS

The term of "air quality models" or "diffusion models" has a wide range of the meanings. For many situations we had better to understand an air quality model as a software which is applied to the air quality predictions. "CDM" or "CRSTER" is not only a nominal to express the scientific means, but also a proper noun. Sometimes these terms mean the trade marks or registered names to be protected from a commercial infringement.

Recently, the quality assurance for software goods became an important concern. The air quality models cannot be an exception. What is the quality for an air quality model? The most important quality characteristic may be the predictive performance, and this performance can be measured by the statistical score obtaind by the measured concentrations and the predicted ones. An example for these evaluation measures is proposed by American Meteorological Society (Fox,1980).

Dekker and Sliggers (1992) discussed the good manufacturing practice for an air quality model. They listed the quality criteria for computer models: 1) mathematical models, 2) software packages, 3) user friendliness, and 4) after sales service. The items 3) and 4) may become important issues for the development of future air quality models.

The air quality models for the Total Pollution Load Control must be validated by the data archives prior to the prediction. This procedure is required by the regulatory laws in Japan, and it may contribute to the quality assurance for the air quality model. However, in case of the air quality models used for environmental assessment, this procedure is not required. Therefore the models without validation were often used for the environmental assessment in Japan.

We have much experience to use the models based on the Gaussian plume equation. However, this does not mean that any specific model based on the Gaussian plume equation used for the specific environmental matter has the good quality for predictive performance, because an air quality model is a composite system which consists of many parts and the basic mathematical expression (for example, Gaussian plume equation) is no more than one component for this system. The good quality must be approved as the total system which includes the plume rise equation, diffusion parameters and a classification scheme for the meteorological conditions. The traceability is also an important factor for the good quality of the air quality models. In order to improve the traceability, the procedure, specification and input data for air quality simulation should be well documented.

Buckley (1991) investigated the accuracy of environmental impact predictions which include air quality, water quality and so on. He pointed out that although there were 800 - 1000 EISs produced in Australia, available articles for evaluation were only 3 %, because the necessary informations were not disclosed. He also concluded that the predictions were less than 50 % accurate on average, and continuing audit of EI prediction is necessary.

There are no reasonable and fixed procedures to evaluate the quality of the air quality models. One of the possible examples may be the system of United States. The text for the quality assurance of the software goods may also be useful to make a system in which the quality of the air quality models is evaluated. Another possible way may be to require that makers of air quality models must take an attestation of the ISO 9000 series quality system.

RESEARCH NEEDS FOR FUTURE PLANNING

In order to contribute to the good environmental management, we must use appropriate air quality models with good quality. This good quality means that the model shows enough high evaluation scores even if the model is applied to many kinds of situations: complex terrain, coastal area and so on. For many areas except Japan we cannot expect the dense network for air monitoring. Therefore the model developed should be already validated with sufficient data archives before regulatory use.

The air quality models supplied should be well documented including computer source code, I/O specifications and the evidence of the good quality. This evidence is given by the evaluation score of predictive performance. A document that states that the data archives used for a model evaluation study have sufficient quality is also necessary.

Unfortunately, it is difficult to find any models with sufficient quality. To make a computer code of an air quality model based on the Gaussian plume equation is not so difficult, but to show that this model has enough performance is very difficult because of the lack of sufficient database.

All stages of the model development should be carried out by qualified contractors which have to take an attestation of the ISO 9000 series quality system. External audit for quality control should also be carried out not only for the field programs but also for the model development and evaluation stage.

CONCLUDING REMARKS

The air quality models belong to the most important tools for an environmental management. The regulatory use of the model is a main topic of this article. There are many papers concerning the scientific or engineering aspects of the air quality modeling. However, only a few papers can be found for the political and economical factors of the air quality models. How to use them or what is their objective became a major concern for the atmospheric modeling.

It is believed that this paper may provide some insights to air quality modeling. In case of the environmental assessment concerning air quality, the most important factor is to use the appropriate air quality model which can be applied to the target emission sources. Since the technological progress produces new types of emission sources, continuous improvement of air quality modeling is also necessary to fulfill the needs of model users.

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