J. KOSAE Vol. 24, No. E2 (2008) pp. 63~73
Journal of Korean Society for Atmospheric Environment

Variation of ANN Model's Predictive Performance Concerning Short-term (< 24 hrs) SO_2 Concentrations with Prediction Lagging Time

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(Received 22 January 2008, accepted 18 September 2008)

Abstract

In this study, neural network models (NNMs) were examined as alternatives to dispersion models in predicting the short-term SO_2 concentrations in a coastal area because the performances of dispersion models in coastal areas have been found to be unsatisfactory. The NNMs were constructed for various combinations of averaging time and prediction time in advance by using the historical data of meteorological parameters and SO_2 concentrations in 2002 in the coastal area of Boryeung, Korea. The NNMs were able to make much more accurate predictions of 1 hr SO_2 concentrations at ground level in the morning in coastal area than the atmospheric dispersion models such as fumigation models, ADMS3 and ISCST3 for identical conditions of atmospheric stability, area, and weather. Even when predictions of 24-h SO_2 concentrations were made 24 hours in advance, the predictions and measurements were in good accordance (correlation coefficient=0.65 for n=216). This accordance level could be improved by appropriate expansion of training parameters. Thus it may be concluded that the NNMs can be successfully used to predict short-term ground level concentrations averaged over time less than 24 hours even in complex terrain. The prediction performance of ANN models tends to improve as the prediction lagging time approaches the concentration averaging time, but to become worse as the lagging time departs from the averaging time.

Key words : Neural network model, Prediction performance, Fumigation model, Complex terrain, Training parameter

1. INTRODUCTION

The closure model like CTDMPLUS (James *et al.*, 1992) and the transport models such as CALPUFF and RAPTAD, which are relevant to the prediction of air pollution dispersion in complex terrain, need three-dimensional windfield data (US EPA, 2000; Tamada *et al.*, 1992; Hanna *et al.*, 1984). There are significant limitations in predicting the short-term air pollution in complex terrains using the popular dispersion models such as ISC, ADMS and AERMOD because these models can not well simulate the complexity of surface roughness and rolling terrain, the spacial inhomogeneity of atmospheric stability along the horizontal plane of the traveling plume, and the unsteady state before sun-rise and after sunset (Christine and John, 2001; Hanna *et al.*, 2001; Boznar *et al.*, 1993). Since horizontal Gaussian distribution of pollution concentrations can not be assumed

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due to slow variations in wind direction over one-hour period during stable conditions (Collet and Oluyemi, 1997), the prediction of air pollution using Gaussian model does not perform well in such cases even in flat terrain. Fumigation models, which were specially formulated to estimate peak ground level concentrations due to frequently occurring fumigation in the morning in coastal area, predict high concentrations better than ISC and ADMS dispersion models do, however, can not predict so accurately (Park and Seok, 2007). Predictions of short-term concentrations using numerical models need high monetary and time costs because of the large temporary variations in the emission and meteorology data and the spatial variations in the terrain data. There are many situations where attaining detailed informations on sources and other parameters such as three-dimensional windfields is difficult.

While linear regression models have been used to cope with the limitations relevant to dispersion models, they do not accurately simulate nonlinear environmental systems (Gardner and Dorling, 1998). Predicting of air pollution concentration using time-series models or a method combining time-series models and dispersion models do not accurately predict peak concentrations (Park and Kim, 1984). Thus, the development of other methodology for predicting the air pollution seems to be necessary so that decisions concerning air pollution source planning can be accurately made. Although artificial neural network (ANN) models may not necessarily solve all of the limitations of traditional statistical models, they provide better approximations than traditional statistical models because they efficiently compute highly dimensional nonlinear data and generalize correct prediction using new input data-sets once computer training has occurred (Chelani *et al.*, 2002; Gardner and Dorling, 1998; Kim and Lee, 1994; Hormik *et al.*, 1989). Chelani *et al.* (2002) compared the predictive performances of a multivariate regression model and an ANN model concerning ground level SO_2 concentrations in the Delhi area, and concluded that the performance of the ANN model, trained with historical data of temperature, relative humidity, wind speed, wind direction and SO_2 concentration, was better than that of the multivariate regression model. There have been several papers reporting the applications of ANN models with multilayer perception to predict ground level ozone concentration (Comrie, 1997; Yi and Prybutok, 1996) and emission rates of pollutants (Rege and Tock, 1996). Although there has been a report that an ANN model can correctly predict ground level SO_2 concentration even when the computer was trained using very limited data (Mok and Tam, 1998), there do not appear to exist any reports concerning how predictive performance varies with the combined conditions of prediction lagging time and averaging time. In this study, the following studies were systematically carried out to develop ANN models being able to predict the short -term ground-level SO_2 concentrations in a complex coastal area where three-dimensional windfield data are not available, but high prediction performance is needed: (i) to select appropriate input variables for the ANN model; (ii) to examine methods for supplementing the missing input data; (iii) to examine how the modeling performances vary with prediction lagging time and averaging time; and (iv) to compare between the predictions of the ground level SO_2 concentration using the ANN models and atmospheric dispersion models.

2. DEVELOPMENT OF ANN MODELS

2.1 Structure and development of ANN models

ANN models consist of input, hidden and output layer to artificially simulate human intelligence, and have been widely used in predicting the future of very nonlinear time series by approximating the relevant functions between input and output variables, and classifying the patterns of both variable. Neural networks are capable of learning many patterns using one or more hidden layers because neurons have nonlinear activation functions (Gardner and Dorling, 1998). Fig. 1 illustrates a structure of a neural network.

In this study, an error backpropagation algorithm was used so that a computerized neural network could learn the patterns that relate the historical data of

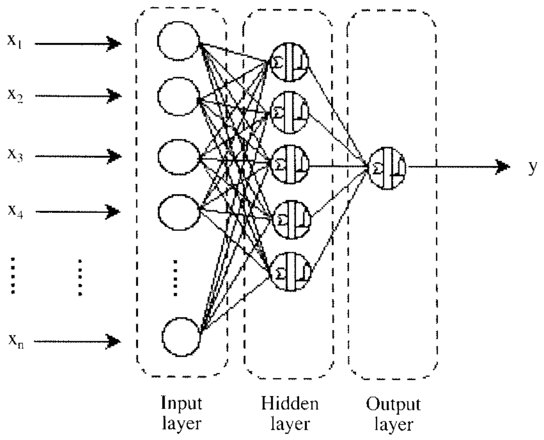


Fig. 1. Structure of a neural network.

independent variables, including meteorological and environmental pararameters, to the dependent environmental variable at lag time. ANN models were constructed by adjusting the initial linkage weights on the basis of errors obtained from the output layer. The procedure of developing an ANN model to predict atmospheric pollution is as follows: (i) to determine the input parameters influencing the level of pollution and the number of nodes of the input layer, (ii) to classify normalized data of meteorological and environmental parameters into a training set (; 70% of normalized data) for computer learning and a test set for confirming the accuracy of the ANN model, (iii) to repeatedly train the computer using the training set so that the errors between the measurements and calculations fall into an appropriate range, and (iv) to recognize the ANN models as a reliable tool for forecasting the environmental concentrations in future once the ANN models are confirmed as an accurate approximator using the test set.

2.2 Preprocessing of input data

Taking the Zannetti *et al.*'s (1976) suggestions concerning meteorological factors influencing the SO_2 concentrations in Venice and the results of such a study in Boryeung into consideration, SO_2 concentrations and meteorological factors, including wind direction, wind speed, temperature and stability, were selected as the input parameters of the ANN models used to predict short-term SO_2 concentrations. The parameter of SO_2 concentration was selected as an independent input variable because it results from the combined effects of meteorology and emission, and contributes as a preceding empirical data to the prediction of the dependent variable. The selection of atmospheric stability differentiates this study from previous relevant reports on ANN model application. Through preliminary study (Sin, 2006), linear and quadratic method were confirmed as being superior to Lagrange and Spline methods in supplementing the missing data of wind direction, wind speed, temperature, and SO_2 concentration, while the Lagrange method was better than the other methods in supplementing the missing data of stability. Thus, the linear method was used to supplement the missing data of wind speed, wind direction, temperature and SO_2 concentration, and the Lagrange method used for stability. The work necessary for supplementing the input missing data was completed before ANN modeling work. Since each input parameter has values (or ranges) and units significantly different from other parameters, all input data were normalized using the Min-Max method (NN Toolbox User's Guide) expressed in equation (1) so that those input variables had converged values ranging from zero to unity.

$$X=\frac{x_i-x_{min}}{x_{max}-x_{min}} \tag{1}$$

where X is a normalized value of the input parameters, and x_i is an input parameter value before normalization.

Since an input parameter such as wind direction with circulating characteristics could be perceived by the neural network as if x° was identical with $(360-x)°$, sigmoid normalization was conducted using equation (2) before loading under considering both the Boznar *et al.* (1993) and Chelani *et al.* (2002). Since the wind rose for the Boryeung area shows that sea breeze from near NW direction could cause fumigation in the coastal area, $(1+\sin\theta)$ instead of $\left[1+\sin\left(\theta+\frac{\pi}{4}\right)\right]$ (Chelani *et al.*, 2002) may be reasonable as a function of wind direction indexing.

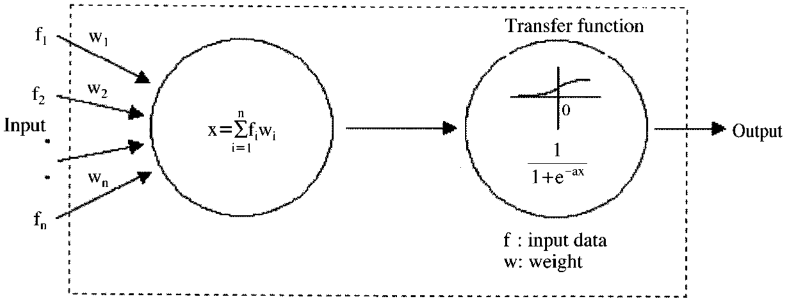


Fig. 2. Neuron computing process.

$$\theta_n=\frac{(\sin\theta_1+1)}{2} \tag{2}$$

Where θ_n is normalized wind direction, and θ_1 is wind direction before normalization (°). $(1+\sin\theta_1)$ is a wind direction index, which can be normalized by dividing with 2 so that resultant θ_n can range from 0 to unity.

2.3 Computer training of ANN models and the testing the training results

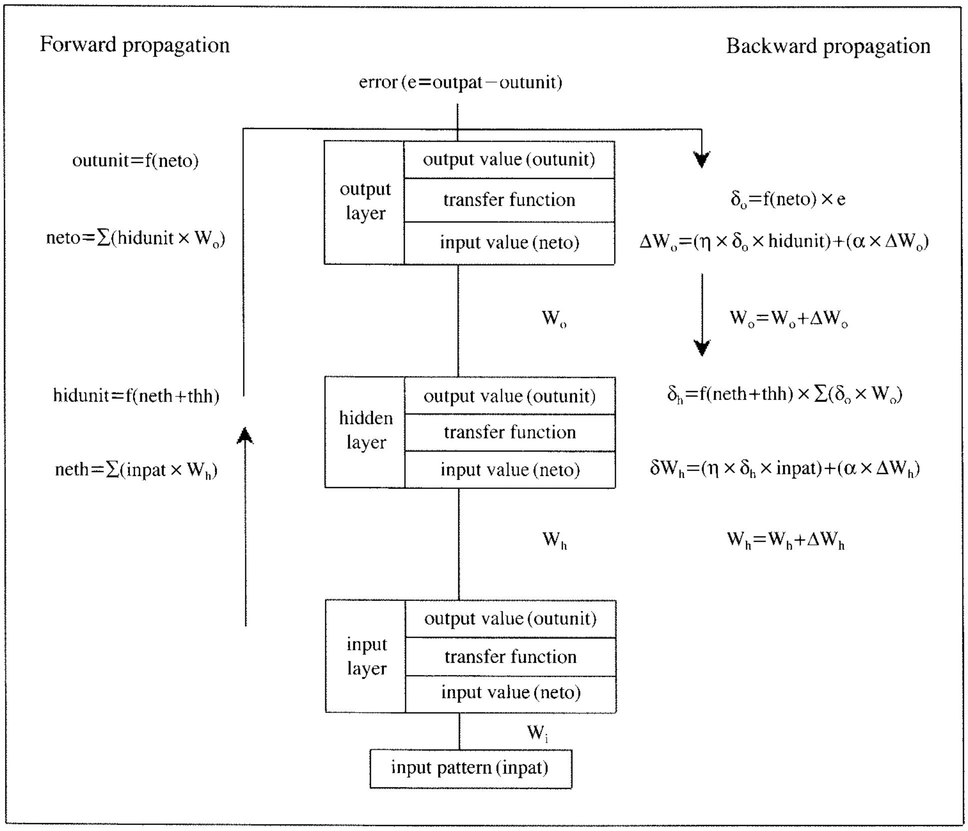
The input data of various parameters were distributed as signals into each neuron of the ANN input layer (Fig. 1) and fed forward via the hidden layer to the output layer, meanwhile the weighted sums of the input data ($x=\sum_{i=1}^{n} f_i \cdot w_i$, where f_i is the ith input data, and w_i is the weight for the ith input data) were received as input by the next layer as shown in Fig. 2. The normalized prediction value of the nonlinear function, $y=\frac{1}{1+e^{-ax}}$ was obtained in the output layer, and the error, e, was calculated by comparing the output value with the normalized measurement value. When the error value was inappropriate, the feedforward networks stored in the computer were trained using the error backpropagation algorithm (Fig. 3) proposed by Bishop (1995). Training was terminated when the error value fell into a satisfactory range after adjusting the linkage weight ($W_h=W_h+\Delta W_h$), because over fitted neural networks might reduce learning error, but could deteriorate the validation of prediction for new input data (Gardner and Dorling, 1998).

The graphical user interface (GUI) was built using the MATLAB® 7.0 neural network toolbox, and used to develop the ANN models in this study. Using the GUI allowed (i) the input data for Boryeung area to be normalized before it was loaded into the computer system, (ii) the structure for a new ANN model to be built, (iii) the number of neurons to be allocated for each layer shown in Fig. 1, (iv) the ANN models to be trained for each averaging time as well as the prediction lagging time, and then (v) the ground level SO_2 concentrations to be predicted for each combinations of averaging time and prediction lagging time after model validation based on the test data set for Boryerng area. Five hundred was assigned as the number of iteration to terminate computer training process after checking the validation error via some trial. The prediction accuracies of the models were tested by comparing the predicted and measured concentratoins, resulting in the adjustment of the linkage weight (e.g., −0.65 for temperature, −6.30 for wind direction, 2.51 for wind speed, 1.80 for stability, and 1.60 for SO_2 concentration in Fig. 4(b)) to improve the performance of the ANN models.

3. USE OF ANN MODELS FOR PREDICTING AIR POLLUTION IN COMPLEX COASTAL TERRAIN

3.1 Terrain, meteorology, and environmental data in the modeling area

A coastal area in Boryeung, Korea was selected as the modeling area for this study. Although there are somewhat objective definitions of complex terrain



inpat	input pattern	h	hidden-layer
outpat	output pattern	o	output-layer
hidunit	hidden-layer output	f	sigmoid function
outunit	output-layer output	net	input of each neuron
W_h	weight from hidden-layer to input-layer	neth	net of hidden layer
W_o	weight from output-layer to hidden layer	thh	threshold of hidden layer
W_i	initial weight		

Fig. 3. Error propagation procedure.

(Choi *et al.*, 2007), coastal area was subjectively defined as a complex terrain in this study in a sense that sea and land, which have very different thermal characteristics, are facing to each other. The following data were available for this area: (i) hourly SO_2 concentration data during Jan. to Dec., 2002 at 11 monitoring sites near the Boryeung power plant, (ii) the emission source data of the power plant, (iii) hourly data of temperature, wind direction, wind speed, relative humidity, and rainfall, (iv) isolation, cloudiness, cloud height, field pressure, and sea level pressure recorded every three hours, and (v) the atmospheric pressure and temperature data at high altitude. Through multiregression analysis, temperature, wind direction, wind speed, and atmospheric stability were identified as effective parameters influencing the SO_2 concentration in the modeling area. The fact that atmospheric stability was taken as an independent parameter in the process of developing ANN models appears to be discriminate from previous works.

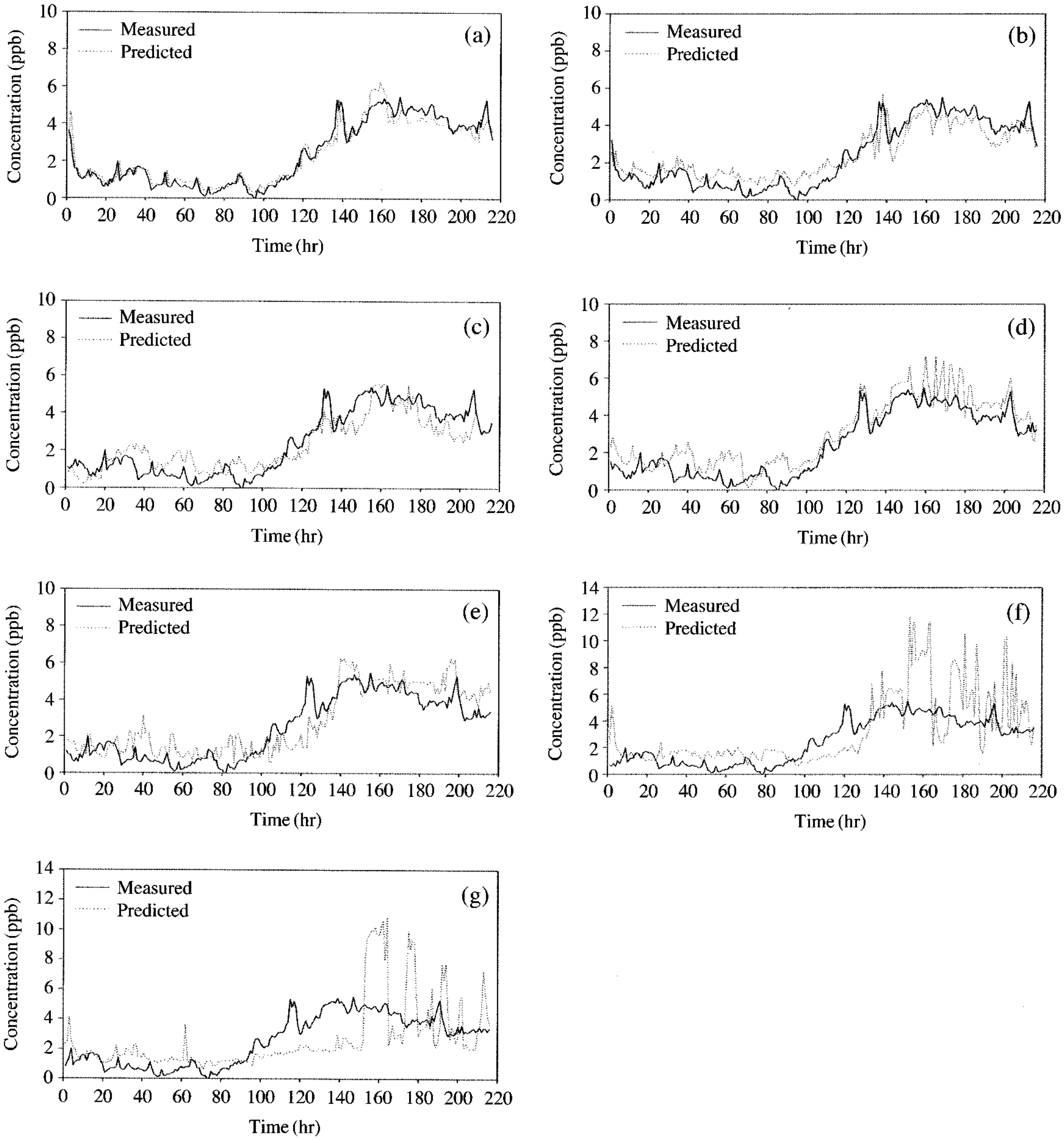


Fig. 4. Time series comparison between measurements and predictions of 1 hr average SO_2 concentrations using neural network models for lagging time of (a) 1 hr, (b) 3 hrs, (c) 8 hrs, (d) 12 hrs, (e) 15 hrs, (f) 18 hrs, and (g) 24 hrs (n=216).

3.2 Modeling results and discussion

3.2.1 Comparing measurements and calculations for various averaging and prediction lagging time

Fig. 4 displays the 1 hr average SO_2 concentrations predicted using the ANN models and the measured concentrations. The ANN models completed the training and testing procedures including the adjustment of initial linkage weights. The correlation coefficients between the predicted and measured SO_2 concentrations were found to decrease as the prediction lagging time exceeds or becomes short

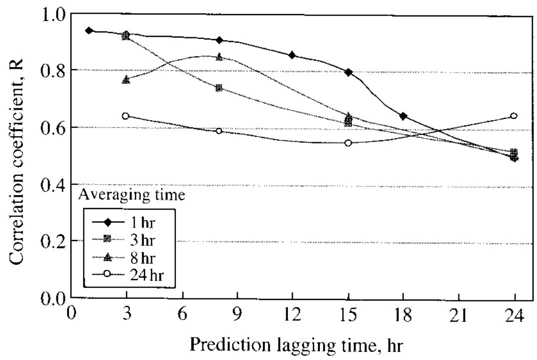


Fig. 5. Variations in correlation coefficients between measurements and predictions of SO_2 concentration with prediction lagging time.

the averaging time as shown in Fig. 5. The decrease in the correlation coefficient appears to be caused due to the increased variations in the emission and weather conditions when the lag time increased. If the lag time exceeded about 12 hours, the performance indices for the averaging time of 1 hr tended to abruptly decrease. This result may probably be due to the 12 hours period of weather change such as the sea/land breeze and stable/unstable condition. There could also be considerable change in emission in addition to the meteorology.

In order to see the effect of the lagging time alteration on the prediction performance of the ANN models, calculations of SO_2 concentration were conducted for various combinations of averaging time and prediction lagging time, and the results were shown in Fig. 6.

Ground level SO_2 concentrations averaged for time periods of 3, 8 and 24 hours were calculated by applying the initial linkage weight obtained for each time period to the ANN models built for the various lagging time. The correlation coefficients and skill scores between the measurements and predictions of 216 pairs are shown in Table 1. The skill score was taken as a fraction of the coincident instances to the total pairs of predictions and measurements when the range of each class for both groups was taken to be 2 ppb.

The skill score of about 0.7 for the large samples (n=216) appears to accord well with the predictions that fall within FAC2 (a factor of two i.e. from 1/2 to 2 times of measurements). The skill score of 0.56 (n=216) for 24 hours of averaging and lagging time appears to be a considerably large value, but corresponds to the smallest value in Table 1. This fact suggests that the ANN models can be used to predict the short-term (averaging time $\leq$ 24 hrs) ground level SO_2 concentrations less than 24 hours in advance even over complex terrain. Considering Table 1, Figs. 4, 5 and 6, it may be concluded that the prediction performance of ANN models tends to decrease as the prediction lagging time exceeds or becomes short the averaging time, but to increase as the lagging time approaches the averaging time.

3.2.2 Predictoin performance comparison between ANN and dispersion models

To investigate the performance of ANN models in a complex coastal area, the 1 hr SO_2 concentration predictions using the ANN and dispersion models were compared at the SONGHAK site around the Boryeung power plant. The dispersion models used in this study were ISCST3, ADMS3, and fumigation model. The model of Lyon and Cole (1973), expressed in equation (3), was confirmed as a fumigation model with good predictability of high SO_2 concentrations at ground level in the morning over coastal area by Park and Seok (2007).

$$C_{(x,\,y)f}=\left\{Q\left[\int_{-\infty}^{p}\frac{1}{\sqrt{2\pi}}\exp(-0.5p^2)dp\right]\Big/ \sqrt{2\pi}\,\sigma_{yf}\cdot\bar{u}\cdot h_i\right\}\cdot\exp(-y^2/2\sigma^2_{yf}) \qquad (3)$$

where $C_{(x,\,y)f}$ is the ground level concentration at (x, y) during fumigation (g/m^3), Q is emission strength (g/s), y is the lateral departure from the plume axis at the downwind distance x from source (m), σ_{yf} is the ground level lateral dispersion coefficient at distance x during fumigation (m), $\bar{u}$ is the mean wind speed within thermal internal boundary layer (TIBL) (m/s), h_i is the thickness of TIBL at distance x from source (m), and p is the difference between h_i and H_e (effective stack height), normalized by σ_z (vertical dispersion coefficient).

The input parameter, $\sigma_{yf(x)}$, was defined by equa-

Table 1. Correlation coefficients and skill scores (in brackets) between measurements and predictions of SO_2 concentrations (ppb) using neural network models (n=216) for various combinations of averaging and lagging time.

Averaging time	Lagging time, hr						
	1	3	8	12	15	18	24
1 h	0.94 (0.88)	0.93 (0.82)	0.91 (0.77)	0.86 (0.76)	0.80 (0.67)	0.65 (0.58)	0.50 (0.51)
3 h		0.92 (0.68)	0.74 (0.70)		0.62 (0.65)		0.52 (0.60)
8 h		0.77 (0.67)	0.85 (0.66)		0.65 (0.73)		0.51 (0.75)
24 h		0.64 (0.71)	0.59 (0.62)		0.55 (0.68)		0.65 (0.56)

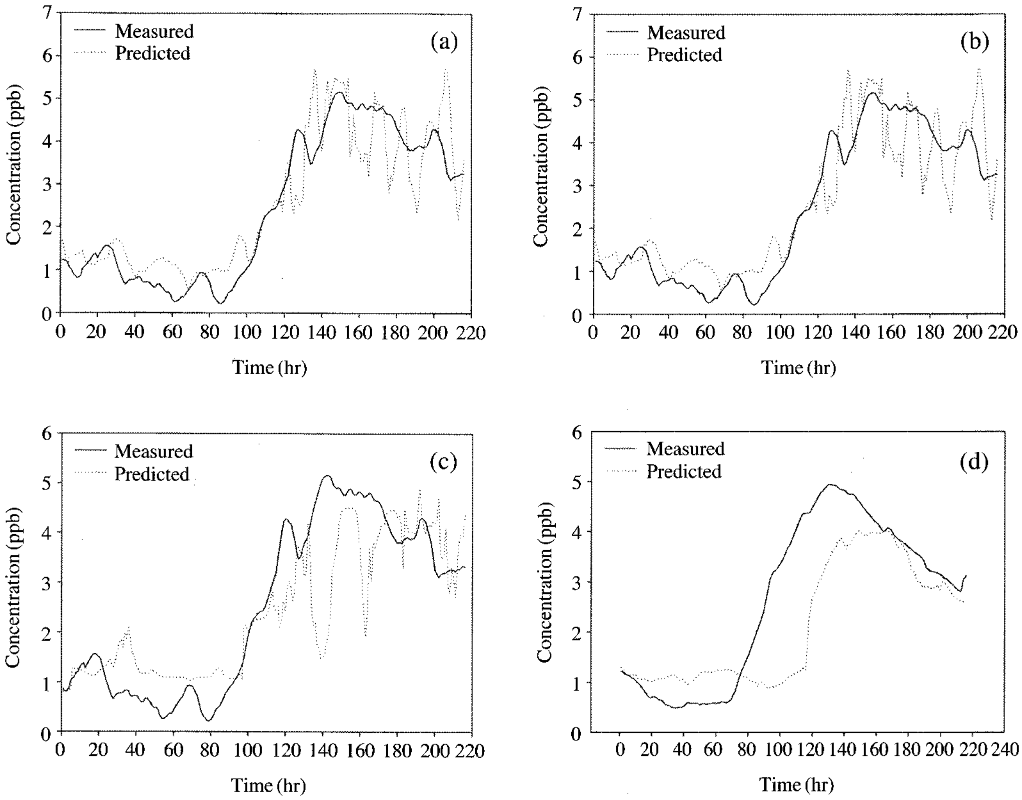


Fig. 6. Time series comparison between measurements and predictions of SO_2 concentrations (ppb) using neural network models for various combinations of averaging time and prediction lagging time (in brackets) of (a) 3 (3) hrs, (b) 8 (8) hrs, (c) 8 (15) hrs, and (d) 24 (24) hrs (n=216).

tion (4) and $\sigma_{y(x)}$ was determined using equation (5) from van Dop *et al.* (1979). These equations (4) and (5) were also recommended by Park and Seok (2007) after evaluation.

$$\sigma_{yf(x)} = \sigma_{y(x)} + H_e/8 \tag{4}$$

$$\sigma^2_{y(x)} = \sigma^2_{ys(x_2)} + \sigma^2_{yt(x)} - \sigma^2_{yt(x_2)} \tag{5}$$

where $\sigma_{y(x)}$ is the lateral dispersion coefficient (m) within TIBL at distance x and height H_e before deposition of plume, σ_{ys} is σ_y (m) in the stable atmospheric layer, and x_2 is the downwind distance (m) for the plume to intersect the top of TIBL.

In order to evaluate the predictions of the ANN and dispersion models in this study, the statistical

Table 2. Statistical measures for the 1 hr SO_2 concentration prediction results of the ANN model and various dispersion models.

Statistical measure	Measure value for perfect modeling	Recommended value of measure	ISCST3 (n=1,820)	ADMS3 (n=700)	Fumigation model (n=230)	ANN model (n=216)
FB	0	$-0.3<FB<0.3$[1]	1.74	−0.85	−0.12	−0.01
MMSE	0	$NMSE<4$[1]	24.75	27.31	1.80	0.04
MG	1	$0.7<MG<1.3$[1]	–	–	2.19	1.12
VG	1	$VG<1.6$[1]	–	–	132.51	1.25
FAC2	1	$0.5 \leq FAC2$[1]	0.003	0.003	0.33	0.94
IOA	1	$0.5 \leq IOA$[2]	0.38	0.01	0.26	0.98
UAPC	0	$-0.2 \leq UAPC \leq 0.2$[3]	−2.45	−12.16	0.07	0.12
MRE	0	$-0.15 \leq MRE \leq 0.15$[3]	0.87	−5.02	−1.03	0.05
R	1	depends on n value	0.03	0.26	0.08	0.93

[1]Chang and Hanna (2004), [2]Zawar-Reza *et al.* (2005), [3]Ziomas *et al.* (1998)

measures proposed by Chang and Hanna (2004), Zawar-Reza *et al.* (2005), and Ziomas *et al.* (1998) were used. Table 2 shows the recommended values of those statistical measures, which were given by these investigators, as well as the values for the models results. The ANN model built for the one-hour average and lag time was used for comparison purpose. The ANN models were manifested to significantly be superior to the dispersion models including fumigation model even in predicting the short-term SO_2 concentrations at ground level in the morning in complex coastal area. Again, the ANN model appears to be superior to other statistical models including regressive method in the prediction of short-term peak concentration.

4. CONCLUSIONS

Multilayer neural network models were built and examined as alternatives to dispersion models in order to improve air pollution predictions over complex coastal terrain. Computer was trained for various combinations of averaging and lagging times by using the historical data of meteorological and environmental parameters for the coastal area around the Boryeung Power Plant. The following conclusions were drawn from the performance investigation of the ANN models:

1) The ANN model's predictions of 1 hr SO_2 concentrations one hour in advance in a complex coastal area were very significantly better in correctness than those of the dispersion models for the same time, area, pollutants and weather.

2) It was possible to make very accurate predictions ($R=0.74$ for $n=216$) of short-term (<8 h) SO_2 concentrations a short time (<8 h) in advance using ANN models built with the historical data of SO_2 concentrations and meteorological parameters including temperature, wind speed, wind direction and atmospheric stability. The coincidence level between the measurements and the predictions of SO_2 concentrations averaged over 24 hours made 24 hours in advance using the ANN models was found to be considerably high ($R=0.65$ for $n=216$). This level could be improved by appropriate selecting the input parameters. Therefore, it may be concluded that ANN models can be used as substitutes for dispersion models in predicting the short-term (≤ 24 h) air pollution levels less than 24 hours in advance even over complex terrain.

3) The prediction performance of ANN models tends to improve as the prediction lagging time approaches the concentration averaging time, but to decrease as the lagging time departs from the averaging time.

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