Ozone Modeling Using Neural Networks

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ABSTRACT

Ozone models for the city of Tulsa were developed using neural network modeling techniques. The neural models were developed using meteorological data from the Oklahoma Mesonet and ozone, nitric oxide, and nitrogen dioxide (NO_2) data from Environmental Protection Agency monitoring sites in the Tulsa area. An initial model trained with only eight surface meteorological input variables and NO_2 was able to simulate ozone concentrations with a correlation coefficient of 0.77. The trained model was then used to evaluate the sensitivity to the primary variables that affect ozone concentrations. The most important variables (NO_2, temperature, solar radiation, and relative humidity) showed response curves with strong nonlinear codependencies. Incorporation of ozone concentrations from the previous 3 days into the model increased the correlation coefficient to 0.82. As expected, the ozone concentrations correlated best with the most recent (1-day previous) values. The model's correlation coefficient was increased to 0.88 by the incorporation of upper-air data from the National Weather Service's Nested Grid Model. Sensitivity analysis for the upper-air variables indicated unusual positive correlations between ozone and the relative humidity from 500 hPa to the tropopause in addition to the other expected correlations with upper-air temperatures, vertical wind velocity, and 1000–500-hPa layer thickness. The neural model results are encouraging for the further use of these systems to evaluate complex parameter cosensitivities, and for the use of these systems in automated ozone forecast systems.

1. Introduction

This paper describes the development of a neural network model for ozone (O_3) for the city of Tulsa, Oklahoma. Such neural models offer a complementary approach to the analysis and prediction of atmospheric ozone from first principles using deterministic or other statistical model systems. The advantage of neural systems is that they are trained using historical data and easily can incorporate complex nonlinear codependent variables (such as temperature and relative humidity). Once trained, the models are not limited severely by spatial or temporal inaccuracies and data gaps. Most important, models trained on specific datasets can be used to evaluate the dependency of a specific parameter under specified conditions [e.g., ozone dependence on nitrogen dioxide (NO_2) within a specified solar radiation, temperature, humidity, pressure, etc.]. The sensitivity analysis for the variables of interest can be very useful for evaluating the type of ozone problem that is present for a particular location. The strength of neural networks lies in their ability to correlate and to display complex nonlinear relationships in a tractable manner.

Ozone concentrations in the southern United States have been described as embedded plumes within a rising tide of ozone (Chameides and Cowling 1995). As such, a considerable amount of the diurnal variation in ozone is dependent on general meterological and wind field

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TABLE 1. Ranges of input parameters for model with surface meteorological data.

Variable	Min	Max	Mean
Relative humidity, % ($\pm$3% estimated)	25	102	79
Temperature of air at 1.5 m, °C	14.3	42.7	26.9
Temperature of air at 9 m, °C	14.0	41.5	26.0
Wind speed at 2 m, m s^{-1}	0.0	8.2	1.9
Wind speed at 10 m, m s^{-1}	0.0	11.3	2.5
Barometric pressure, hPa	984	1002	993
Solar radiation, W m^{-2}	0	1035	258
Ozone, ppb	0	104	38
NO, ppb	2	121	3
$NO_{2,}$ ppb	1	59	6

conditions. For the current model, the surface meteorological input is obtained from the Tulsa County Bixby site of the Oklahoma Mesonet. The Mesonet is a distributed network of weather monitoring sites in each county of Oklahoma (Brock et al. 1995). (At the time of writing, readers could find out more about the Oklahoma Mesonet by visiting the Oklahoma Climate Survey Web site at ocs.ou.edu.) Air quality data are provided by a longitudinal network of three O_3 and two nitrogen oxides [$=NO_x$ = nitric oxide (NO) + NO_2] monitoring sites in and around Tulsa County extending from the rural southern sections through the city to the rural northern sections, as established by the EPA. (Maps and more detailed information are available at the time of writing through the Oklahoma Department of Environmental Quality Tulsa County Air Quality web site at http://204.87.67.183.) In this work, data from the Bixby Mesonet and Environmental Protection Agency (EPA) monitoring sites for the summer of 1996 were used. The mean O_3 level for the summer of 1996 fell within the range of 37–42 ppb for the three EPA ozone monitoring locations.

2. Database

The O_3, NO, and NO_2 data (Table 1) consisted of hourly averages recorded at the monitoring stations (site 174—Glenpool, site 137—Skiatook, and site 127—Mohawk Park). These data were obtained from the Aerometric Information Retrieval System (AIRS), the U.S. Environmental Protection Agency (EPA) air quality database.

The surface meteorological data (Table 1) used in the neural network model came from the Oklahoma Mesonet Bixby site in southern Tulsa County. This network provides wind speed and temperature at two heights, solar radiation, relative humidity, wind direction, soil temperature, and other parameters. Some of the parameters are available at 5-min intervals and others at 15-min intervals.

3. Neural network model

A neural network can be defined as a distributed computational system composed of a number of individual processing elements operating largely in parallel, interconnected according to some specific topology (architecture), and having the capability to self-modify connection strengths during the processing of element parameters (learning) (Haykin 1994). Figure 1 shows a simple feed-forward neural network used in this work. The neural network model was developed using the Pro-

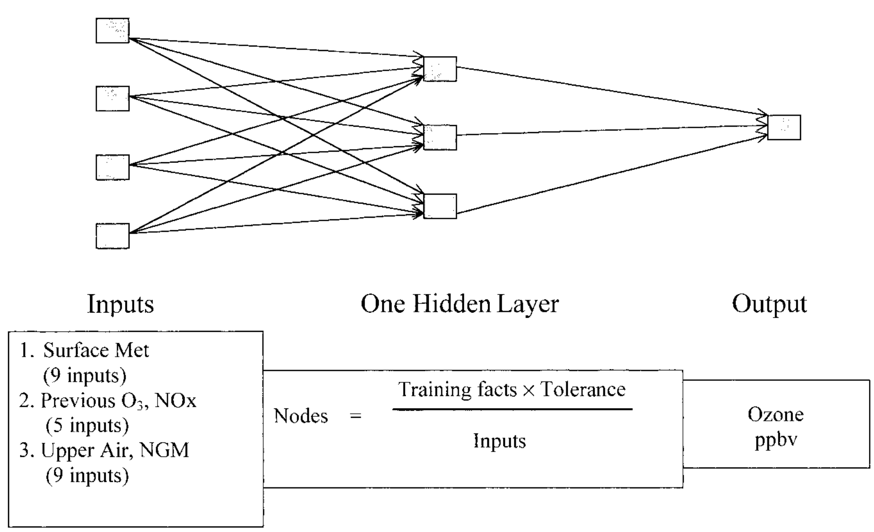

FIG. 1. Simple feed-forward neural network. Input nodes (or neurons) use time-synchronous data that can include surface and upper-air meteorological parameters as well as chemically speciated NO_X and ozone concentrations for the previous days. The number of nodes in the single hidden layer depends on the number of input neurons. Training occurs through back propagation, which changes the internodal connection strengths to minimize the difference in the observed ozone output node.

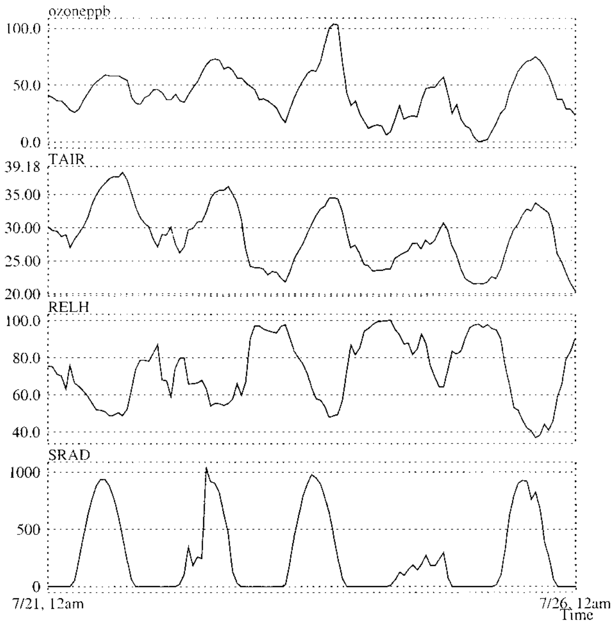

FIG. 2. Typical time series example for model inputs and observed ozone. Ozone concentrations (ppb) for a 5-day period (local time) are shown along with TAIR (air temperature at 9 m; °C), RELH (relative humidity; %), and SRAD (solar radiation; W m^{-2}).

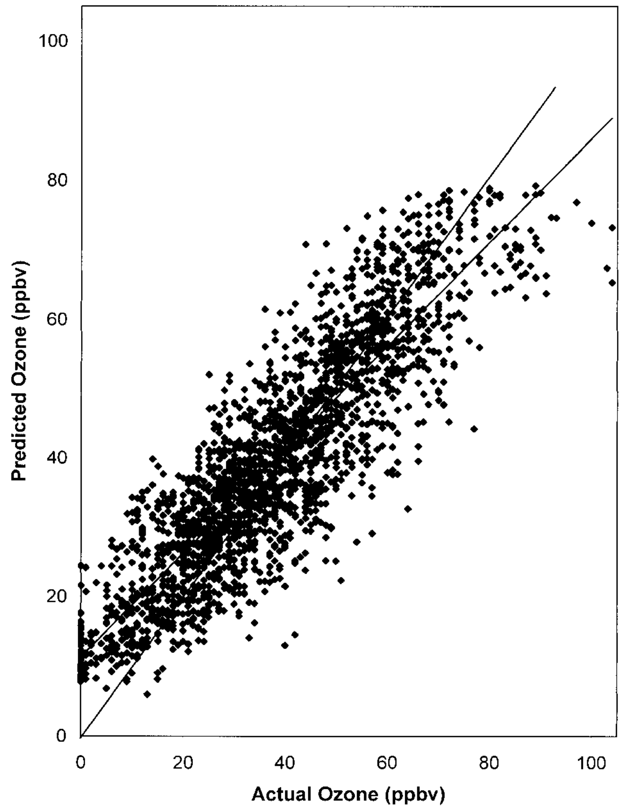

FIG 3. Observed vs predicted ozone concentration for model with only surface meteorological data and NO_2. An R^2 value of 0.77 was observed.

cess Insights software package developed by Pavilion Technologies, Inc. The prediction model uses a feed-forward neural network with casual connectivity. The architecture was set never to allow any connections to go backward in time. With the inputs and outputs coincident in time, this architecture is a simple three-layer feed-forward neural network with linear units on the input layer and sigmoidal units on the hidden and output layers.

The EPA AIRS and the Mesonet data needed extensive formatting and transforming to enable the dataset to be read into Process Insights. This reformatting was done using Microsoft Excel with the supporting Visual Basic programming for multitasking operations. Process Insights also has several built-in tools for data transformation and formatting, which were used to make the datasets further suitable for training purposes.

The raw data for O_3 and NO_x from the EPA AIRS were in intervals of 1 h and the raw meteorological data from the Mesonetwork were in intervals of 5 and 15 min. The dataset had to be time merged before it could be used with the Process Insights model. The data had to be made row synchronous (i.e., all data rows of the file were associated with the same time), and any time delay between rows was adjusted. Time merging converted each dataset to this required format by expanding and averaging the data as necessary. Time merging also filled in data to replace points that were deleted or missing. The built-in time-merge tool in Process Insights was used for this purpose.

4. Results and discussion

The parameters that were used as inputs for the simplest model were NO and NO_2 (ppb), temperature of air at a height of 9 m (°C), temperature of air at a height of 1.5 m (°C), solar radiation in (W m^{-2}), relative humidity (%), wind speed at a height of 10 m (m s^{-1}), wind speed at a height of 2 m (m s^{-1}), and station local barometric pressure (hPa). Table 1 gives the statistics for the different variables used in the model. In Fig. 2 the typical correlation between the predominant meteorological parameters and the observed ozone concentrations are displayed for a 5-day period. A positive correlation between O_3 and temperature or solar radiation is shown clearly, whereas a negative correlation is observed for relative humidity (or dewpoint, not shown).

This first model was trained using the dataset that contains only the nine surface variables. A randomly selected set consisting of 15% of the total samples in the dataset was used for testing. The model gave an R^2 of 0.77 for all data points. The R^2 value can be interpreted as the proportion of the variance in the simulated values attributable to the variance in the actual values. A comparison of the model's simulated output values with the actual output values is seen in Fig. 3. Note that

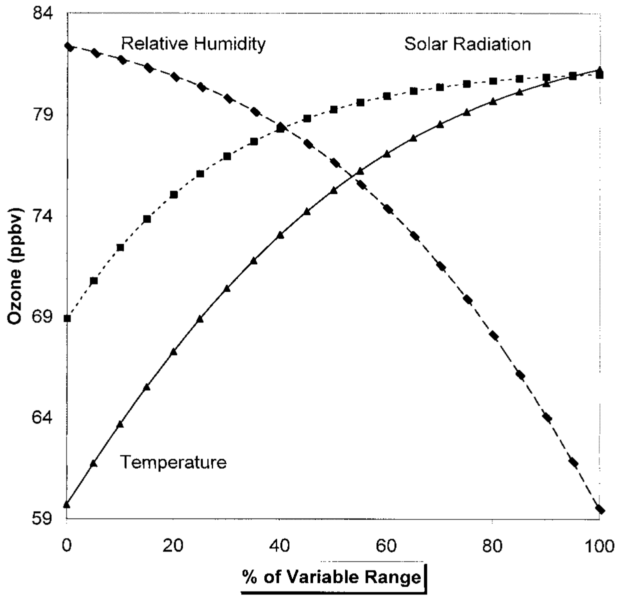

FIG. 4. Model outputs for ozone concentration vs temperature, solar radiation, and relative humidity. For the temperature sensitivity plot, ozone model output was determined as the temperature at 1.5 m was increased across its range of values for summer 1996 from 14.3° to 42.7°C. Solar radiation and relative humidity (RH) were held constant at 950 W m^{-2} and 40.1%, respectively. All other parameters are fixed at the respective mean values. For the solar radiation sensitivity plot, ozone model output was determined as solar radiation ranged from its minimum value of 0 to its maximum value of 1035 W m^{-2}. Air temperature was held constant at 40°C and RH was kept at 40.1%. For the RH sensitivity, the parameter was varied from its minimum value of 24.5% to its reported maximum, uncorrected value of 101.5%, as air temperature and solar radiation were kept constant at 40°C and 950 W m^{-2}, respectively, and all other parameters were at their mean values.

the model fails to reproduce certain points toward the higher end of the ozone range. These points were not scattered over the entire summer but appeared on only five specific days. The model underestimated the O_3 trends on these days; these days essentially were different from the remaining days that were estimated more closely. It is possible that the ozone trend on these days was influenced by a parameter not featured in the inputs to the model and related to either a vertical mixing parameter or a long-distance transport factor.

Once trained, all parameters can be fixed to determine the selective dependence on a single input. For example, Fig. 4 shows the details of how O_3 varies across the range of temperature, solar radiation, or relative humidity when the other parameters are fixed. The calculations are made by stepping each variable through its range while holding all other variables at a fixed value. In Fig. 4, temperature was varied, while the relative humidity and solar radiation were kept constant at 35% and 950 W m^{-2}, respectively. These values were chosen to represent typical values for a somewhat dry, sunny day, which has a moderately high O_3 potential. For the other curves, temperature was held constant at 40°C, while the respective parameter was varied.

As expected, when temperature and solar radiation increase, O_3 concentrations increase. Note, however, that the temperature and solar radiation curves flatten out near the higher end of their ranges, and the nonlinearity is greater for solar radiation (Fig. 4). Considering that the photolysis of NO_2 to NO and atomic oxygen is the most important reaction responsible for ozone production, beyond a certain threshold of radiation, NO_2 photolysis may not be the limiting factor for ozone production. Further increases in radiation intensity contribute less appreciably to O_3 production. In contrast to temperature, relative humidity shows a more linear negative correlation. The reciprocal trends between temperature and relative humidity thus exhibit a similar, but not completely complementary, dependence. The equivalent trend also is seen using dewpoint rather than relative humidity (not shown). Moisture in the air may enhance the removal of O_3 and hydroperoxy radicals (Colbeck and MacKenzie 1994). Ozone production also is reduced as its precursors NO and NO_2 react with water to form soluble acids such as nitrous acid. In addition, a moist atmosphere inherently is less stable than a dry atmosphere, and therefore vertical motions may be enhanced, resulting in greater dispersion of pollutants.

To gain further insight into the dependence of O_3 concentrations on the meteorological parameters, the model was trained with the inclusion of other parameters such as ΔT, the difference between the temperature at 9 m and 1.5 m. Figure 5 shows the variation of O_3 across the range of ΔT. It can be seen from the figure that for values of ΔT less than 50% of its range, O_3 has a very low sensitivity to ΔT. However, as ΔT increases above 50% of its range, it has a more pronounced effect on O_3. When ΔT increases, the upper-air temperature is greater than the lower-air temperature. This condition suppresses vertical motions caused by buoyancy and helps to form a stable layer of air, thus subduing the dispersion of pollutants.

Figure 6 demonstrates how the model can be used to evaluate the effects of a particular component in O_3 production. The two curves show the ozone produced as NO_2 varies from 2 to 30 ppb with all the other parameters fixed except dewpoint. As shown in the upper curve, the production of O_3 is less dependent on the NO_2 concentrations at a dewpoint of 16°C. When the dewpoint is increased to 29°C, however, the production of O_3 is more dependent on the NO_2 concentrations. This behavior could be caused by the presence of alternative sinks for NO_x at high moisture levels, making O_3 production more NO_x limited.

Past work in the literature has suggested that ozone episodes are usually multiday events (Feister and Balzer 1991). This duration means that there is a gradual buildup of ozone concentrations, leading to the occurrence of an ozone episode. This behavior prompted use of ozone concentrations from preceding days as an input

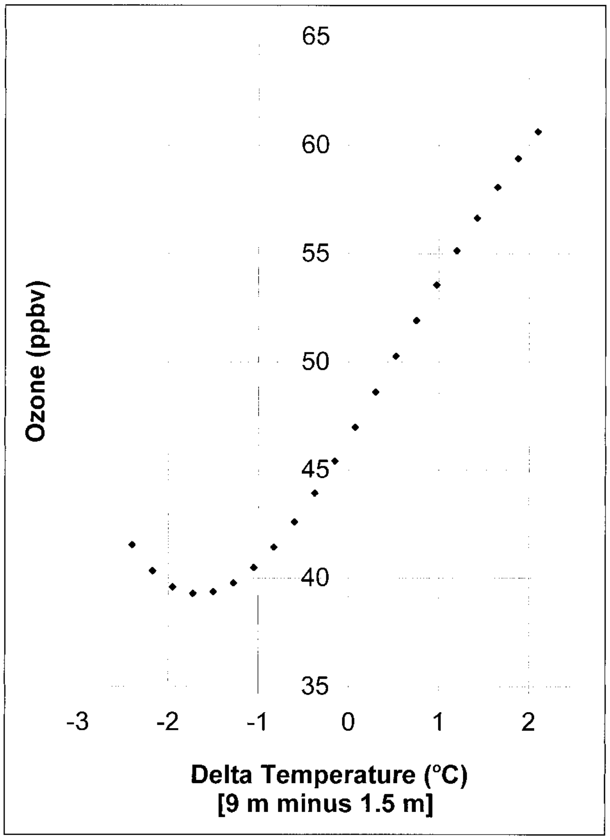

FIG. 5. Ozone concentration vs ΔT. The sensitivity for ΔT (9-m minus 1.5-m temperatures; °C) was evaluated across its range of values for summer 1996. Positive values for ΔT correspond to a stable atmosphere. All other parameters were held at the mean values.

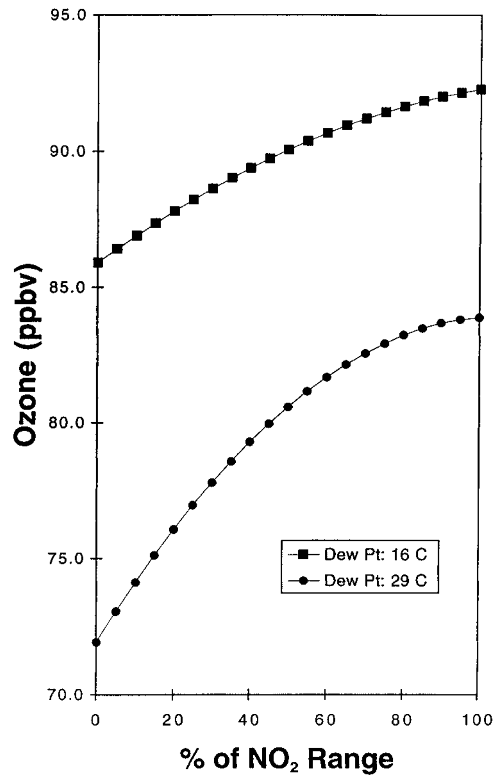

FIG. 6. Ozone concentration as a function of NO_2 concentration with respect to changes in dewpoints (Dew Pt; °C).

to the model. Three different input variables, each representing hourly concentrations of ozone from one of the previous 3 days, were included as inputs to the model, and the model was retrained. Therefore, for each concentration of ozone at a particular time of the day as an output, there are three inputs, each representing the ozone concentration at the same time on each of the previous 3 days. The model R^2 went up from 0.77 to 0.82, with all three variables having a positive correlation. The current ozone concentrations correlated best with those from 1 day back, and the correlation diminished with those from 2 and 3 days back. In a way, this result supports the multiday event theory. The meteorological conditions responsible for an ozone episode usually are persistent for a few days before their ozone-forming potential diminishes.

While O_3 concentrations are affected by surface meteorological parameters, they are known to be affected by upper-air parameters also (Bloomfield et al. 1996). The thermal and frictional forces from the earth's surface cause large diurnal changes in the depth of the planetary boundary layer, from hundreds of meters at night to several kilometers during the day. Therefore the upper-air parameters play an important role in the dispersion and transport of ozone and its precursors. Upper-air parameters obtained from the National Weather Service's Nested Grid Model (NGM) were included in the neural network model. Time-zero observations from the NGM for the parameters shown in Table 2 were used as inputs.

The model was retrained after inclusion of the above parameters. The model R^2 went up from 0.82 to 0.88. A comparison of the model's simulated values and the actual output values is shown in Fig. 7. It can be seen that the simulation accuracy of the model has improved

TABLE 2. NGM parameters used as inputs in the neural network model.

NGM variable	Description
T1	Temperature (°C) of model layer 1, 35-hPa thickness starting from the surface
T2	Temperature (°C) of model layer 3 at 900 hPa
T3	Temperature (°C) of model layer 5 at 800 hPa
R1	Relative humidity (%) of model layer 1, 35-hPa thickness starting from the surface
R2	Relative humidity (%) of model layers 2–9, from 35 hPa above the surface to 500 hPa
R3	Relative humidity (%) of model layers 10–13, from 500 hPa to the tropopause
VVV	Vertical wind velocity at 700 hPa (10^{-3} hPa s^{-1})
HH	1000–500-hPa thickness (dm)
LI	Four-layer lifting index (°C)

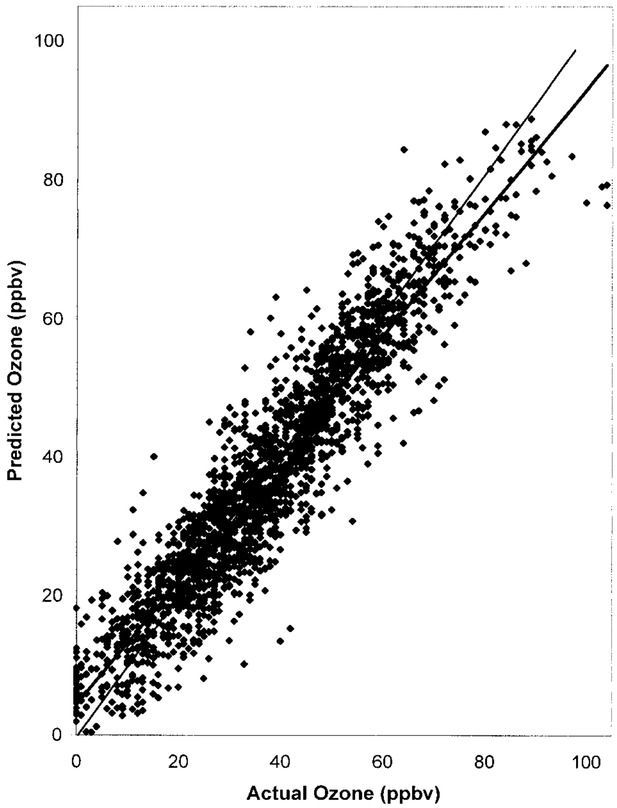

FIG. 7. Observed vs predicted ozone concentration for model with the incorporation of upper-air meteorological data, 3 previous days' ozone concentrations, and ground-level meteorological data.

substantially from that of the model with just surface meteorological parameters included. The model still severely underpredicts the ozone concentrations on 2 days.

From the sensitivity analyses of the model parameters, it was observed that, among the upper-air parameters, the ozone concentrations were sensitive to the relative humidity from 500 hPa to the tropopause. It is remarkable that the relative humidity at such a height could correlate with ground-level ozone concentration. The temperature at three heights, relative humidities at the other two heights, thickness of the layer from 1000 to 500 hPa, and vertical wind velocity (Table 2) also correlated with ozone concentrations. Lifting index had a poor correlation with ozone concentration.

5. Summary and conclusions

These early results of the model are encouraging, especially considering the fact that data for volatile organic compounds were not used. The correlation between observed and predicted ozone concentrations increased from an R^2 of 0.77 with surface parameters only, to 0.82 with the three previous days' ozone concentrations, to 0.88 with upper-air NGM input. The model can be used to gain insight into the typical nonlinearity involved in the process and to evaluate each parameter's sensitivity. These analyses are relatively easy to obtain using neural network models.

Additional developments of the model are under way to include soil temperature, soil moisture, wind direction, and rain events. The neural network model also is being modified to make 8-h average simulations of ozone in accordance with the new National Ambient Air Quality Standard, which considers an 8-h average of 80 ppb or greater to be an ozone exceedance. Some of the preliminary work in this direction has shown better success than for the 1-h averages, and a more extended model is being tested and trained on data from multiple summers. At present, the model is being used in a forecast mode to provide officials in Tulsa with 8-h average predicted ozone concentrations. The results from summer 1998 currently are being evaluated.

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