Short-Range Prediction of Tropospheric Ozone Concentrations and Exceedances for Baton Rouge, Louisiana

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ABSTRACT

Previous research has been focused on improving forecasts of the daily maximum 1-h concentration of tropospheric ozone, which was based on criteria used by the U.S. Environmental Protection Agency (EPA). However, in 2001, EPA began implementing standards based on daily maximum 8-h mean concentrations rather than the former 1-h period. This study uses principal components analysis and multiple-regression analysis to forecast daily maximum 8-h ozone concentrations in the Baton Rouge, Louisiana, nonattainment zone. Although model performance for values at individual stations proved unsuccessful, likely because of the effects of local nonmeteorological conditions, a model for prediction of ''exceedances'' of the standards at three or more stations explains 46.2% of the variance in tropospheric ozone concentrations. Furthermore, a decision-making tree is proposed for short-range forecasting of whether an exceedance is expected. Results represent a first attempt to forecast 8-h peak tropospheric ozone concentrations for this region.

1. Introduction

Previous research has analyzed the spatial and temporal characteristics of tropospheric ozone ''exceedances'' in the Baton Rouge, Louisiana, nonattainment zone (Fig. 1) according to the new national ambient air-quality standard of 85 ppb averaged over an 8-h period (cf. the previous one-hour 125-ppb standard) being implemented by the U.S. Environmental Protection Agency (EPA) (R. Rohli et al. 2003, unpublished manuscript, hereinafter RHB). Results suggested that the new regulations will increase the number of exceedances, and the spatial pattern of exceedances may be explained at least partially by diurnal phenomena and synoptic weather patterns (RHB). The purpose of this research is to develop multiple regression and ''decision tree'' models for forecasting ozone exceedance days in the Baton Rouge area. Although similar techniques have been attempted elsewhere, no formal meteorological study has focused on modeling ozone concentrations or exceedances in the Gulf Coast region of the United States under the revised EPA thresholds.

Several attempts to model ozone concentration using regression techniques (e.g., Comrie 1997; Hubbard and Cobourn 1998; Chaloulakou et al. 1999; Draxler 2000; Ryan et al. 2000), neural networks (e.g., Comrie 1997; Soja and Soja 1999; Spellman 1999), three-dimensional transport and dispersion models (e.g., Draxler 2000), and airmass-based trajectory analysis (e.g., Comrie 1994; Cobourn and Hubbard 1999) have been performed. Regression studies have shown reasonable fits between predicted and observed ozone concentrations. Neural-network techniques offered only slight improvement over regression models. Transport and airmass trajectory methods have generally been the least successful. Nevertheless, prediction of exceedance days using the former 1-h standard met with only limited success (e.g., Ryan 1995; Hubbard and Cobourn 1998). Efforts to model exceedances under the revised 8-h standard

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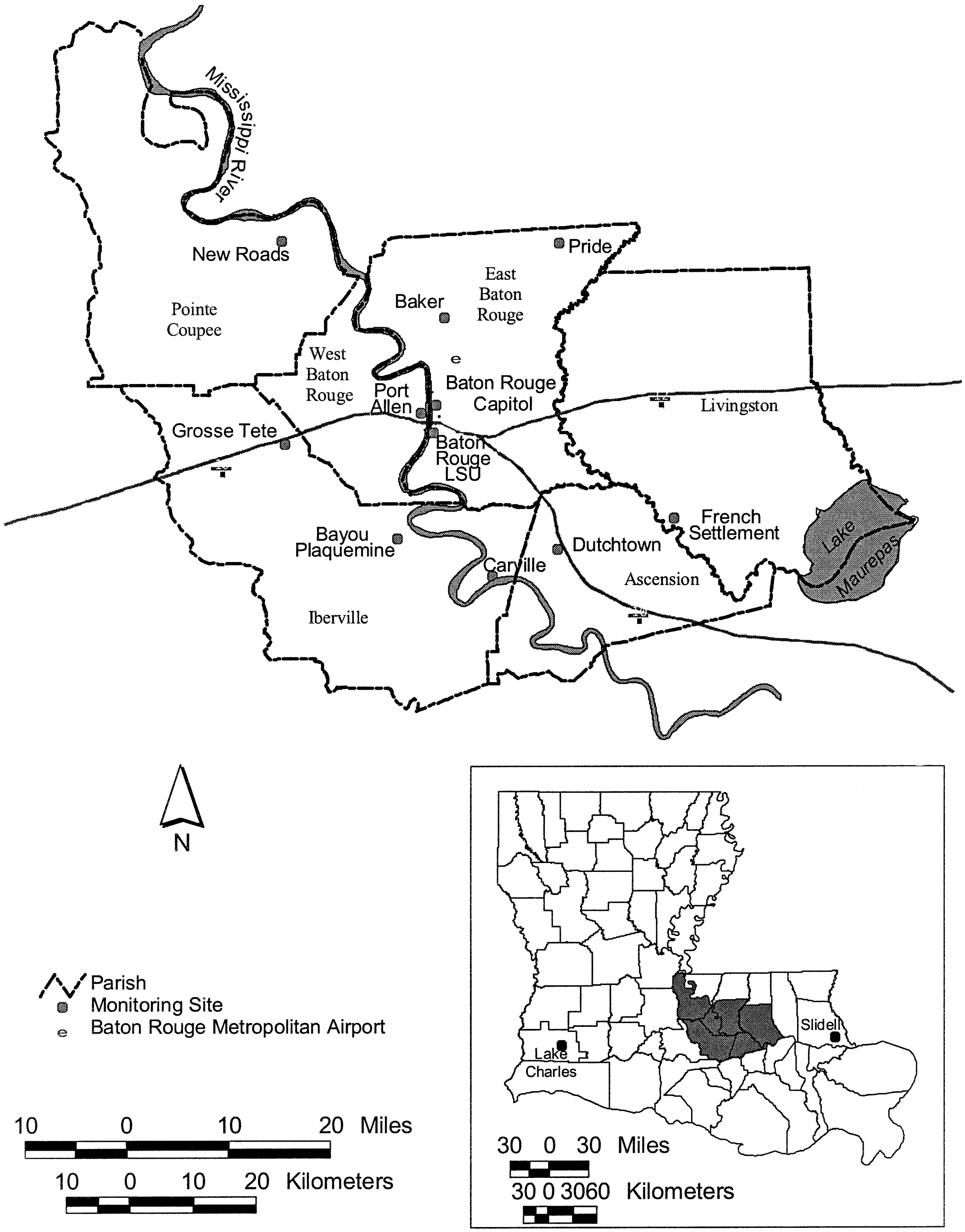

FIG. 1. The Baton Rouge, LA, ozone nonattainment zone.

are even more challenging (and largely untested in the refereed literature) because a concentration near 85 ppb through the diurnal cycle may be caused by relatively unspectacular weather conditions, as compared with the distinct atmospheric features that would be necessary to cause concentrations to exceed 125 ppb. Thus, ‘‘the difference in weather conditions between eight-hour exceedance and non-exceedance days will be slight and likely more difficult to forecast’’ than 1-h exceedance days (U.S. EPA 1999).

2. Data and methods

a. General data collection and processing

A methodology identical to that of RHB is employed here. Hourly tropospheric ozone concentrations for the 11 sites in the Baton Rouge nonattainment zone (Fig. 1) were obtained for the 1995–99 period of record [M. Vanichchagorn, Louisiana Department of Environmental Quality, 2001, personal communication]. In addition, 2000 data were used to test the model. In general, less than 5% of the observations were missing at each station. Missing data from 2200 to 0600 LST were ignored, because tropospheric ozone is not problematic at these hours. For days having one missing observation between 0700 and 2100 LST, linear interpolation was used from adjacent temporal observations to ''fill in'' the missing datum. Days having more than one missing observation between 0700 and 2100 LST were discarded from analysis.

b. Statistical modeling of ozone concentrations

Four families of variables are included in the pool of possible predictors, and they are based on recommendations of common predictor variables used to forecast ozone concentrations (U.S. EPA 1999). The first is 0700 LST surface data measured by the Automated Surface Observation System at Baton Rouge Metropolitan Airport (hereinafter referred to as BTR; Fig. 1). These data are considered ''official'' measurements, are readily available on a near–real time basis on the Internet, and include surface air temperature T_a, dewpoint temperature T_d, dewpoint depression $T_a - T_d$, wind speed W, west–east (u) and south–north (v) wind components, sea level pressure P, and visibility. The second category of variables includes maximum T_a on the exceedance day and on the day prior to the exceedance day at BTR. The former is represented by the forecast high T_a for that day in model applications and is the only predicted value among our pool of possible ozone predictors. The third set of variables involves chemical constituents of the atmosphere. These are represented by the maximum 0700 LST measured nitrogen oxides (NO_x) concentration among the 11 sites and the peak ozone concentration at any site on the day prior to the relevant day. The final family of potential predictor variables includes upper-air data from 1200 UTC on the morning of the day in question. In particular, 850- and 700-hPa temperature, 500-hPa heights, and 1000-hPa u and v wind components are included. These variables represent vertical mixing features, synoptic-scale weather features, and transport from upwind regions, respectively. Because the nearest official National Weather Service radiosonde stations are located at Lake Charles and Slidell (Fig. 1), the mean of each of the upper-air variables at these two sites is used to represent the value over Baton Rouge.

Because of high multicollinearity among independent variables, multiple-regression equations using an all-inclusive approach for independent variable selection would be biased. Therefore, a principal components analysis (PCA) is performed (Dunteman 1989) as a data-reduction technique (e.g., Kalkstein and Corrigan 1986; Yarnal 1993), using the entire pool of input variables on each day that has at least one observation of at least 85 ppb. The Baker site (Fig. 1) is chosen to represent the Baton Rouge nonattainment zone for this part of the analysis because of its proximity to Metropolitan Airport and its suburban location (which represents a compromise between the rural and urban sites). The purpose is to identify those variables that show strong loadings (i.e., correlations between the original variable and the component) on each of the components that explain the greatest amount of variance. These variables are to become potential predictors in subsequent multiple-regression analysis. The method employed here is similar to the factor analytic technique employed by Spichtinger et al. (1996).

PCA is a multivariate quantitative technique whereby eigenvector techniques are used to provide a parsimonious explanation of variability in a dataset on the basis of a few underlying dimensions, or ''modes of variability'' (Dunteman 1989). Although other useful applications of PCA exist, a major application (including that employed here) is as a data-reduction technique. The input data structure for the PCA is ''P mode'' (Richman 1986), in that the temporal observations form the rows and the variables form the columns. The loadings matrix takes the form of variables along the x axis and component loadings along the columns.

The identification of the major modes of variability in this complicated dataset allows for the detection of the variables that are most closely associated with the modes of variability in the dataset. These are the variables that are to be included in the multiple-regression analysis. Because the components are orthogonal to one another in any unrotated PCA procedure, multicollinearity among those variables that load highly on the most important components is minimized. Although orthogonal rotations would retain this property, no rotation is implemented because PCA is purely a data-reduction technique here, and therefore the unrotated solution produces the most parsimonious explanation of the data. Rotation departs from this property and therefore degrades the results (Yarnal 1993). This technique is advantageous over simply including the n variables that have the highest Pearson correlation coefficients to 8-h ozone concentrations because each subsequent component explains ''new'' variance that is unaccounted for by the other components. Therefore, each included variable should have an important role in the model.

At first, days that had at least one hourly observation of 85 ppb at any one site were used in the computation of the multiple-regression equation. However, low explained variances resulted, perhaps because it is possible that local nonmeteorological factors (such as industrial plant emissions) may have produced anomalously high

TABLE 1. Proportions of explained variance by the first 5 (of 17 total) principal components for Baker.

Principal component	Proportion of explained variance	Cumulative proportion of explained variance
1	0.280	0.280
2	0.158	0.438
3	0.103	0.541
4	0.071	0.612
5	0.066	0.678

ozone concentrations at small spatial (i.e., one site) and temporal (i.e., for a 1- or 2-h period rather than for an 8-h period) scales and spared the remainder of the study area from high concentrations. Therefore, only days with a peak mean 8-h concentration of 85 ppb at three sites or more are considered in the generation of the multiple-regression equation. These days are ones in which atmospheric features are assumed to exert a detectable signature using quantitative techniques. Thus, this analysis examines the region as a whole and produces a uniformly applicable equation for predicting maximum ozone concentration in the region. Days for which the predicted value falls somewhat below the 85-ppb threshold might be considered to be meteorologically ''borderline'' days that could produce an exceedance at one site in the study area. In such instances, individual philosophy about the ramifications of issuing ozone alerts, along with the number of previous exceedances in the current season, should serve as the guiding principles for whether an alert should be issued by meteorological consultants and whether human activities should be restricted.

c. *Criteria method of prediction*

Because of the relatively low explained variance using the EPA-recommended variables as a starting point in the statistical model, a decision-tree model is also constructed for use in conjunction with the statistical model. This ''criteria method of prediction'' is most useful for nominal-scale ozone exceedance forecasting (U.S. EPA 1999). Descriptive statistics, particularly the minimum (maximum) threshold of meteorological variables, are noted, so that a decision tree for forecasting of zone exceedances can be created based on thresholds of atmospheric properties of historical exceedances.

The small number of observations by month at each site is problematic. At Pride (Fig. 1), for instance, there are only one, two, three, one, one, seven, and one exceedances in April–October, respectively. Even the site with the most 8-h exceedances (Carville) has only 0, 2, 7, 12, 13, 7, and 0 exceedances in April–October, respectively. Because of the small number of observations in each month, the decision tree applies only for exceedance days anywhere in the region; no attempt is made to create a decision tree for each site. Although surface meteorological observations are taken at each of the ozone monitoring sites, these data are not used for the statistical or decision-tree modeling because they are not official, are limited by local micrometeorological conditions, are not sites for which meteorological forecasts are made, and are not readily available on a near–real time basis. Therefore, surface meteorological data for Metropolitan Airport (Fig. 1) are used in lieu of these data in the predictive equation and decision tree.

3. Results and discussion

a. *Multiple-regression-based modeling of ozone concentrations*

Results of PCA suggest that the first 5 of the 17 total components collectively explain 67.8% of the dataset variance at Baker (Table 1). Subsequent components show a sharp drop in explained variance as indicated by a scree plot, and these are deemed insignificant for the purpose of data reduction. Of the 17 input variables, those having the strongest loadings by component are T_a, $T_a - T_d$, W, P, and maximum NO_x level, all at 0700 LST (Table 2). These independent variables offer some advantages for predictive purposes, such as the fact that they are all measured (rather than forecast) by 0700 LST each day (thereby allowing for a reliable input for forecasting conditions of that afternoon). Also, the first four variables come from the same source (BTR), and these data are reliable, free, and accessible via the Internet on a near–real time basis. No upper-air data are required, so that no interpolation between Slidell and Lake Charles data is necessary. NO_x data are required for the model but are somewhat more problematic, because these data are not routinely available on a timely basis to ozone forecasters/environmental consultants. However, the importance of NO_x for modeling ozone in Ba-

TABLE 2. Variables displaying the strongest loadings by retained component (with loadings shown in parentheses) for Baker. Local NO_x level is calculated at Baker, mean 700-hPa height is calculated as the mean from Lake Charles and Slidell, and all other variables are measured at Baton Rouge Metropolitan Airport.

Principal component	Variable with strongest loading	Variable with second-strongest loading
1	0700 LST temperature (0.414)	Max temperature on the forecast day (0.410)
2	0700 LST dewpoint depression (0.440)	0700 LST visibility (0.437)
3	0700 LST wind speed (0.487)	0700 LST V (−0.495)
4	0700 LST sea level pressure (0.613)	1200 UTC mean 700-hPa height (0.253)
5	0700 LST local NO_x level (0.421)	0700 LST U (0.420)

Table 3. Regression parameter estimates and beta weights for multiple-regression equation to predict 8-h peak ozone concentration at Baton Rouge (y intercept is -1431.745).

Variable	Parameter estimate	Sample std dev	Beta coefficient
Forecast max temperature (°F)	3.904 254	3.899	1.499
Max temperature on previous day (°F)	−1.211 810	4.7896	−0.572
0700 LST air temperature (°F)	−0.726 710	6.047 67	−0.433
Sea level pressure (hPa)	1.311 225	2.2215	0.287
0700 LST wind speed (kt)	1.090 123	1.991	0.214
Max NO_x (ppb)	0.066 593	26.435 96	0.173
0700 LST dewpoint depression (°F)	−0.319 818	2.7192	−0.086
Predictand (max 8-h O_3 concentration)	—	10.154 106	—

ton Rouge cannot be overlooked, because the transport and accumulation of ozone and precursor NO_x from upwind sites, especially on the stagnant western sides of surface anticyclones, plays a potentially important role in the occurrence of exceedance days over Baton Rouge. Similar difficulties in ozone prediction would be expected to occur in other locations downwind from similar industrial sites.

A total of 41 days experienced 8-h exceedances at three or more stations during the 1995–99 period. Multiple-regression analysis using independent variables that represented each of the retained components identified a predictive equation with parameter estimates as shown in Table 3 and a y intercept of -1431.745. The beta weights shown in Table 3 are calculated as the parameter estimate times the ratio of the sample standard deviation for that variable to the sample standard deviation of the predicted variable, and these weights confirm the results from Table 2 that temperature variables are the most important predictors.

In the equation, T_a, $T_a - T_d$, W, and P are all measured at 0700 LST at BTR, and the afternoon high on the day in question is used as the forecast maximum T_a. Of course, imprecise temperature forecasts will reduce the accuracy of the model. The last two terms were included, despite the fact that they did not display the highest loadings, because they improved the adjusted explained variance in the model. These implicitly indicate the importance of persistent warm temperatures in maximizing ozone concentrations. The regression equation (with an intercept term of -1431.75) explains 46.2% of the dataset variance while maximizing the adjusted r^2 value of 0.344. Beta weights range from a minimum absolute value of 0.173 (NO_x maximum value) to a maximum absolute value of 1.499 (maximum temperature on the afternoon of the exceedance).

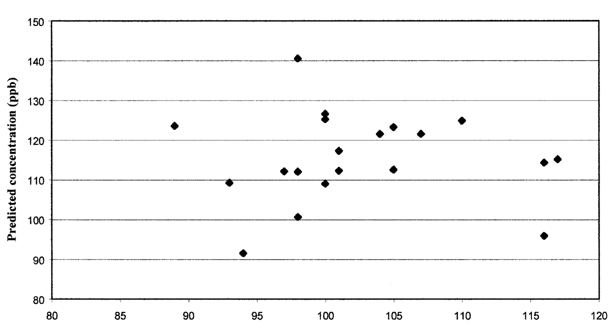

Fig. 2. Scatterplot of predicted vs observed ozone concentrations on days having 8-h concentrations of 85 ppb or more at three or more sites for 2000.

b. Regression model verification

Data for the 20 days in 2000 that had 8-h concentrations of at least 85 ppb at three or more sites were all predicted as exceedances by the regression model, but the model provided a root-mean-square error (rmse) of 18.8 ppb (with overestimation of actual values in 16 of the cases), as compared with an rmse of only 8.3 ppb for the 1995–99 data. A scattergram of the data points is shown in Fig. 2. Nonmeteorological and/or nonlocal factors may be important in producing exceedances (especially in 2000), and the quantitative model is inadequate in some cases. Moreover, the problem of timely acquisition of NO_x data may make this a somewhat unrealistic predictor variable for inclusion in a model. Therefore, an additional approach is taken in an attempt to forecast maximum ozone concentrations more effectively.

c. Meteorological thresholds of exceedances and the decision-tree model

An understanding of the meteorological properties on exceedance days may allow for improvements in forecasting exceedances through the use of a decision tree. Ozone exceedances (at any station) under the proposed standard have occurred on 119 days having the meteorological conditions at Metropolitan Airport summarized in Table 4 (excepting the two events in March). These can be compared to analogous conditions on all April–October days from 1995 to 1999 in Baton Rouge (Table 5). Of course, caution should be exercised in the interpretation of results from this comparison (particularly from using descriptive statistics that imply normal distributions), because of the very small number of observations during 8-h exceedance days in many months shown. Because in this part of the analysis an exceed-

TABLE 4. Surface atmospheric conditions at Baton Rouge Metropolitan Airport on 8-h exceedance days at any station, 1995–99.

		0700 LST temperature (°F)	0700 LST dewpoint depression (°F)	0700 LST surface wind speed (kt)	0700 LST sea level pressure (hPa)	Max temperature (°F)
Apr (n = 3)	Avg	59.7	4	3.3	1018.3	82.3
	Std dev	8.3	4	3.1	4.8	6.1
	Min	53	0	0	1012.8	77
	Max	69	8	6	1021.3	89
	Avg − 2 std dev	43.0	0	0	1008.8	70.1
	Avg + 2 std dev	76.3	12	9.4	1027.8	94.6
May (n = 14)	Avg	66.9	3.7	2.3	1017.4	87.1
	Std dev	4.8	3.3	1.9	2.4	3.2
	Min	58	0	0	1013.2	80
	Max	74	13	4	1022.7	92
	Avg − 2 std dev	57.2	0	0	1012.5	80.8
	Avg + 2 std dev	76.6	10.2	6.2	1022.2	93.5
Jun (n = 15)	Avg	73.9	4.3	2.3	1015.5	90.6
	Std dev	4.1	3.1	2.3	3.2	2.9
	Min	67	0	0	1009.5	85
	Max	81	11	5	1020.1	95
	Avg − 2 std dev	65.8	0	0	1009.2	84.7
	Avg + 2 std dev	82.0	10.6	6.8	1021.9	96.5
Jul (n = 19)	Avg	77.7	3.4	1.9	1016.3	93.7
	Std dev	2.1	1.9	2.0	2.0	2.6
	Min	74	1	0	1011.3	89
	Max	81	8	5	1019.5	100
	Avg − 2 std dev	73.5	0	0	1012.3	88.5
	Avg + 2 std dev	81.9	7.1	5.9	1020.2	98.9
Aug (n = 33)	Avg	76.2	3.5	1.8	1015.4	94.9
	Std dev	3.5	2.0	2.0	1.8	3.1
	Min	64	0	0	1012.7	87
	Max	81	9	6	1019.1	100
	Avg − 2 std dev	69.2	0	0	1011.8	88.7
	Avg + 2 std dev	83.3	7.6	5.8	1019.0	101.2
Sep (n = 25)	Avg	68.8	3.8	1.9	1015.4	92.4
	Std dev	4.5	2.8	2.1	2.6	3.0
	Min	56	1	0	1009.2	83
	Max	78	11	7	1019.7	97
	Avg − 2 std dev	59.7	0	0	1010.2	86.3
	Avg + 2 std dev	77.8	9.4	6.2	1020.5	98.4
Oct (n = 8)	Avg	60.0	2.3	0.9	1017.6	85.4
	Std dev	8.1	1.0	1.6	3.4	5.1
	Min	50	1	0	1014.4	79
	Max	72	4	4	1024.8	93
	Avg − 2 std dev	43.7	0.2	0	1010.8	75.2
	Avg + 2 std dev	76.3	4.3	4.2	1024.4	95.5

ance day is defined as any day in which *any* station reports 85 ppb or more over an 8-h period, all days with an exceedance at any station are included in the analysis. It is obvious from Fig. 3 that the frequency of exceedances by month increases substantially from the former to the present standard.

Comparison of Tables 4 and 5 and examination of the characteristics of the individual exceedances reveal that the 0700 LST T_a is likely to be near or below the monthly normal (with 79 of 113 exceedance days following this pattern and 4 days reporting missing data), $T_a - T_d$ is likely to be at or above normal (71 of 113 cases with 4 days of missing data), and W should not be stronger than normal in order to produce an exceedance (with 96 of 114 days following this pattern and 3 days reporting missing data). In each month, even though the previous day's mean maximum T_a must be relatively high (not shown), the mean maximum T_a on the exceedance day was at least as high as that of the prior day in 92 of the 117 days. Furthermore, the day's maximum T_a was at or above normal in 96 of 117 cases. It is noteworthy that no exceedance has occurred from 1995 to 1999 when W exceeded 7 kt.

As was discussed previously, an insufficient number of events exist to include monthly thresholds for exceedances at each station. Nevertheless, for comparison, meteorological properties during exceedance events are shown for Baton Rouge Capitol (Fig. 1) in Table 6. Baton Rouge Capitol was selected for this analysis because of its relatively high number of events and its proximity to the airport and to the sites that produce the greatest number of exceedances. Much like the com-

Table 5. Atmospheric conditions on all days by month in Baton Rouge, 1995–99.

		0700 LST temperature (°F, BTR)	0700 LST dewpoint depression (°F, BTR)	0700 LST surface wind speed (kt, BTR)	0700 LST sea level pressure (hPa, BTR)	0700 LST max NO_x concentration at any site (ppb)	Max temperature (°F, BTR)
Apr (n = 148)	Avg	60.7	3.6	5.0	1016.0	43.5	77.4
	Std dev	8.7	3.9	3.3	4.9	34.7	6.8
	Min	40	0	0	1002.8	11	58
	Max	76	18	16	1027.4	204	91
	Avg − 2 std dev	43.4	0	0	1006.3	0	63.8
	Avg + 2 std dev	78.1	11.5	11.6	1025.8	112.8	91.0
May (n = 152)	Avg	70.3	2.8	4.2	1015.7	39.6	85.8
	Std dev	5.6	2.8	3.0	3.8	24.2	4.5
	Min	54	0	0	1005.5	11	74
	Max	81	19	13	1027.6	190	97
	Avg − 2 std dev	59.2	0	0	1008.1	0	76.8
	Avg + 2 std dev	81.5	8.3	10.2	1023.3	88.1	94.8
Jun (n = 149)	Avg	75.6	3.1	4.3	1015.6	38.2	89.6
	Std dev	4.2	2.1	3.1	3.1	20.0	4.0
	Min	64	0	0	1006.7	8	75
	Max	84	11	15	1022.3	135	97
	Avg − 2 std dev	67.2	0	0	1009.3	0	81.6
	Avg + 2 std dev	84.0	7.4	10.5	1021.8	78.1	97.5
Jul (n = 153)	Avg	78.3	3.1	3.6	1017.1	36.8	91.8
	Std dev	2.8	1.9	2.8	2.6	21.4	3.2
	Min	71	0	0	1010.1	7	80
	Max	83	11	13	1023.4	180	100
	Avg − 2 std dev	72.7	0	0	1011.9	0	85.4
	Avg + 2 std dev	83.9	6.8	9.3	1022.2	79.7	98.3
Aug (n = 150)	Avg	76.7	3.1	2.9	1016.1	43.3	92.4
	Std dev	3.0	2.0	2.6	2.4	20.1	3.9
	Min	68	0	0	1010.8	12	80
	Max	83	9	9	1021.1	127	100
	Avg − 2 std dev	70.7	0	0	1011.3	3.1	84.5
	Avg + 2 std dev	82.7	7.1	8	1020.9	83.5	100.2
Sep (n = 147)	Avg	70.9	3.5	3.8	1014.5	45.0	88.7
	Std dev	5.4	3.4	3.1	3.1	35.7	5.1
	Min	54	0	0	1003.7	7	69
	Max	81	21	16	1020.8	286	97
	Avg − 2 std dev	60.1	0	0	1008.2	0	78.4
	Avg + 2 std dev	81.8	10.2	10.0	1020.8	116.5	99.0
Oct (n = 153)	Avg	60.9	3.2	4.1	1018.3	53.5	80.1
	Std dev	9.4	3.2	3.1	4.3	41.3	7.0
	Min	38	0	0	1000.0	11	56
	Max	76	16	12	1028.4	232	93
	Avg − 2 std dev	42.0	0	0	1009.6	0	66.2
	Avg + 2 std dev	79.7	9.6	10.2	1027.0	136.2	94.0

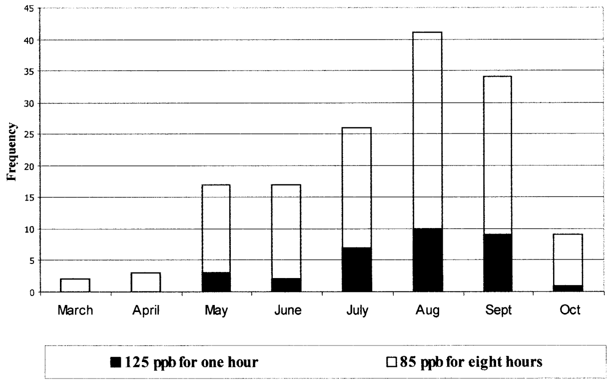

FIG. 3. Number of days exceeding the former and current EPA-standard ozone concentrations in the Baton Rouge area for 1995–99.

posite analysis for exceedances at any station, comparison of Tables 5 and 6 reveals that 8-h exceedances at Capitol are associated with somewhat cooler- and drier-than-normal 0700 LST conditions, light winds, and near-normal *P*. Of course, implementation of descriptive statistics using such low numbers of observation again invites extreme caution in the interpretation of results.

Table 7 shows the criteria meteorological properties, by month, of days with at least three 8-h station exceedances. Results reemphasize the characteristics noted previously. In particular, to have a meteorologically favorable situation for producing exceedances at three or more stations on a given day, morning conditions should be neither warmer nor have smaller dewpoint depressions than normal for that month. In addition, afternoon temperature conditions on multistation exceedance days not surprisingly tend to be higher than normal. Furthermore, the most striking characteristic of three- (or more) station exceedance days is the high 0700 LST NO_x concentrations in the region.

A convenient method of summarizing the characteristics presented in Tables 4–7 is through the use of a decision tree. The decision-tree algorithm for forecasting whether a given day will produce an ozone exceedance at three stations or more is shown in Fig. 4. The tree was devised by the identification of minimum/maximum thresholds of various atmospheric variables that are representative of all the exceedance events at three or more stations. Of course, in some cases, local meteorological and nonmeteorological factors may produce a violation at one or two stations that is undetectable in this kind of analysis.

After validating the model using 2000 LST data, it was found that the decision tree was overestimating the number of ozone days in the region. Inclusion of synoptic weather types and relative humidity was unsuccessful in improving this prediction tool. However, inclusion of the binary ''rain/no-rain on the previous day'' variable was found to improve the forecasting accuracy of the decision-making tree in a simple analysis. Test cases of 12 measured exceedance days using the new criterion from May through August 2000 were examined. It is noteworthy that no measurable rainfall fell at BTR on the day prior to the exceedance day on any of these occasions. Furthermore, 11 randomly selected, nonexceedance days in 2000 that exceeded the high-temperature threshold in the decision-making tree were selected from this time period. All 11 days would have been forecast incorrectly as ozone exceedance days without the ''previous day rainfall'' condition included, but inclusion of this variable would have cut the number of misses by four. Therefore, this simple analysis suggests that if the previous day experienced precipitation anywhere in the region, a ''no'' forecast should be issued. Even though the number of test cases is small, evidence suggests that this condition may provide some improvement in the qualitative model, and the ''was previous day dry'' criterion is included in the flow chart (Fig. 4).

Another important stipulation in the decision tree was that if the 0700 LST *W* at BTR was above 7 kt, an exceedance was still possible (provided the other criteria in the tree were still met) only if the 925-hPa wind speed at Baton Rouge exceeded the wind speed at both the surface and 850 hPa. This condition was included because it was found that a low-level nocturnal jet may be transferring momentum to the surface during some mornings, and this surface wind speed was disqualifying some days from being forecast as ozone days. In reality, however, such a nocturnal jet would disappear by that afternoon, thereby decreasing the surface wind speed to such a level that it would be conducive to ozone loadings. For these upper-air data, all Baton Rouge wind speeds are approximated as the mean speed at Lake Charles and Slidell for the relevant level.

d. Validation of decision-making tree for forecasting an ozone exceedance day

The forecasting success of the decision-making tree is shown in Table 8. Accuracy assessment using the data in Table 8 can be quantified using several indicators (Aguado and Burt 2001). The first is the hit rate, which simply identifies the percentage of correct forecasts. From Table 8, it is apparent that the hit rate is (14 + 112)/153, or 82.4%. Somewhat similar is the probability of detection, which quantifies the accuracy of predicting an exceedance day when one actually occurs (Aguado and Burt 2001). The probability of detection is 14/21, or 66.7%. This number is important because it shows the accuracy of forecasting true exceedance days so that mitigation measures can be undertaken in advance of the event. Of course, because the probability of detection could reach 100% simply by forecasting each day as an exceedance, a measure of the false positives is also important. This is the false-alarm rate and is computed as the proportion of ''yes'' forecasts that were incorrect (Aguado and Burt 2001). In the tree, the false-alarm rate was a high 20/34, or 58.8%. Public alerts or

TABLE 6. Atmospheric conditions on 8-h exceedance days at Baton Rouge Capitol site, 1995–99.

		0700 LST temperature (°F, BTR)	0700 LST dewpoint depression (°F, BTR)	0700 LST surface wind speed (kt, BTR)	0700 LST sea level pressure (hPa, BTR)	0700 LST NO_x concentration (ppb, Capitol)	Max temperature (°F, BTR)
Apr (n = 0)	Avg	—	—	—	—	—	—
	Std dev						
	Min						
	Max						
	Avg − 2 std dev						
	Avg + 2 std dev						
May (n = 4)	Avg	63.5	6.8	1.8	1016.6	41.5	86.8
	Std dev	4.9	4.5	2.1	1.5	17.8	2.8
	Min	58	3	0	1014.6	24	84
	Max	69	13	4	1017.9	61	90
	Avg − 2 std dev	53.6	0	0	1013.6	5.9	81.2
	Avg + 2 std dev	73.4	15.8	5.9	1019.6	77.1	92.3
Jun (n = 5)	Avg	73.6	4.8	1.6	1015.3	72.8	91.6
	Std dev	3.9	4.9	2.3	1.6	42.9	3.0
	Min	68	0	0	1013.6	35	88
	Max	77	11	5	1017.6	135	95
	Avg − 2 std dev	65.8	0	0	1012.1	0	85.5
	Avg + 2 std dev	81.4	14.6	6.2	1018.5	158	97.7
Jul (n = 4)	Avg	76.8	5.0	3.3	1016.4	36.5	93.3
	Std dev	1.0	2.9	0.5	1.6	20.1	1.5
	Min	76	2	3	1014.9	18	92
	Max	78	8	4	1018.0	62	95
	Avg − 2 std dev	74.8	0	2.3	1013.2	0	90.3
	Avg + 2 std dev	78.7	10.9	4.3	1019.6	76.8	96.3
Aug (n = 11)	Avg	76.4	2.8	0.8	1015.5	47.2	95.5
	Std dev	2.3	1.8	1.4	2.0	21.8	3.1
	Min	73	0	0	1013.0	23	90
	Max	80	6	3	1019.1	100	100
	Avg − 2 std dev	71.8	0	0	1011.5	3.7	89.2
	Avg + 2 std dev	81.0	6.4	3.6	1019.5	90.7	101.7
Sep (n = 8)	Avg	69.1	4.4	1.8	1015.6	45.3	92.9
	Std dev	1.9	2.5	2.7	2.3	18.6	1.6
	Min	66	1	0	1012.3	17	91
	Max	72	7	7	1018.6	76	96
	Avg − 2 std dev	65.4	0	0	1010.7	8.0	89.8
	Avg + 2 std dev	72.9	9.4	7.1	1019.9	82.5	96.0
Oct (n = 0)	Avg	—	—	—	—	—	—
	Std dev						
	Min						
	Max						
	Avg − 2 std dev						
	Avg + 2 std dev						

TABLE 7. Atmospheric conditions on days with an 8-h mean concentration of at least 85 ppb at three or more stations, 1995–99.

		0700 LST temperature (°F, BTR)	0700 LST dewpoint depression (°F, BTR)	0700 LST surface wind speed (kt, BTR)	0700 LST sea level pressure (hPa, BTR)	0700 LST max NO_x station concentration (ppb, any station)	Max temperature (°F, BTR)
Apr (n = 0)	Avg	—	—	—	—	—	—
	Std dev						
	Min						
	Max						
	Avg − 2 std dev						
	Avg + 2 std dev						
May (n = 4)	Avg	64.3	5.8	0.8	1017.6	56.3	88.0
	Std dev	5.6	5.6	1.5	0.8	13.6	2.8
	Min	58	0	0	1016.4	42	84
	Max	69	13	3	1018.3	73	90
	Avg − 2 std dev	53.0	0	0	1015.9	29.0	82.3
	Avg + 2 std dev	75.5	17.0	3.8	1019.2	83.5	93.7
Jun (n = 5)	Avg	71.6	3.4	2.4	1016.1	77.6	91.0
	Std dev	4.3	3.5	2.3	2.4	33.6	3.4
	Min	67	0	0	1014.0	53	87
	Max	76	9	5	1020.1	135	95
	Avg − 2 std dev	63.0	0	0	1011.4	10.5	84.2
	Avg + 2 std dev	80.2	10.4	7.0	1020.8	144.7	97.8
Jul (n = 8)	Avg	76.5	4.3	2.8	1016.6	47.0	93.0
	Std dev	1.9	2.3	1.8	1.6	20.0	2.2
	Min	74	2	0	1014.6	27	90
	Max	80	8	5	1019.0	88	97
	Avg − 2 std dev	72.8	0	0	1013.4	7.0	88.6
	Avg + 2 std dev	80.2	8.8	6.4	1019.9	87.0	97.4
Aug (n = 10)	Avg	76.2	2.9	0.9	1015.5	59.8	95.6
	Std dev	2.4	1.9	1.4	2.1	28.7	3.3
	Min	73	0	0	1013.0	34	90
	Max	80	6	3	1019.1	127	100
	Avg − 2 std dev	71.4	0	0	1011.2	2.4	89.1
	Avg + 2 std dev	81.0	6.7	3.8	1019.8	117.2	102.1
Sep (n = 12)	Avg	70.0	4.0	1.7	1014.5	59.0	93.1
	Std dev	3.7	2.2	2.3	2.5	20.8	2.1
	Min	64	1	0	1009.2	18	90
	Max	78	7	7	1018.6	93	97
	Avg − 2 std dev	62.7	0	0	1009.4	17.5	89.0
	Avg + 2 std dev	77.3	8.4	6.3	1019.6	100.5	97.2
Oct (n = 2)	Avg	57.5	3.5	2.0	1016.4	100.5	83.5
	Std dev	3.5	0.7	2.8	1.1	41.7	2.1
	Min	55	3	0	1015.6	71	82
	Max	60	4	4	1017.1	130	85
	Avg − 2 std dev	50.4	2.1	0	1014.2	17.1	79.3
	Avg + 2 std dev	64.6	4.9	7.7	1018.5	183.9	87.7

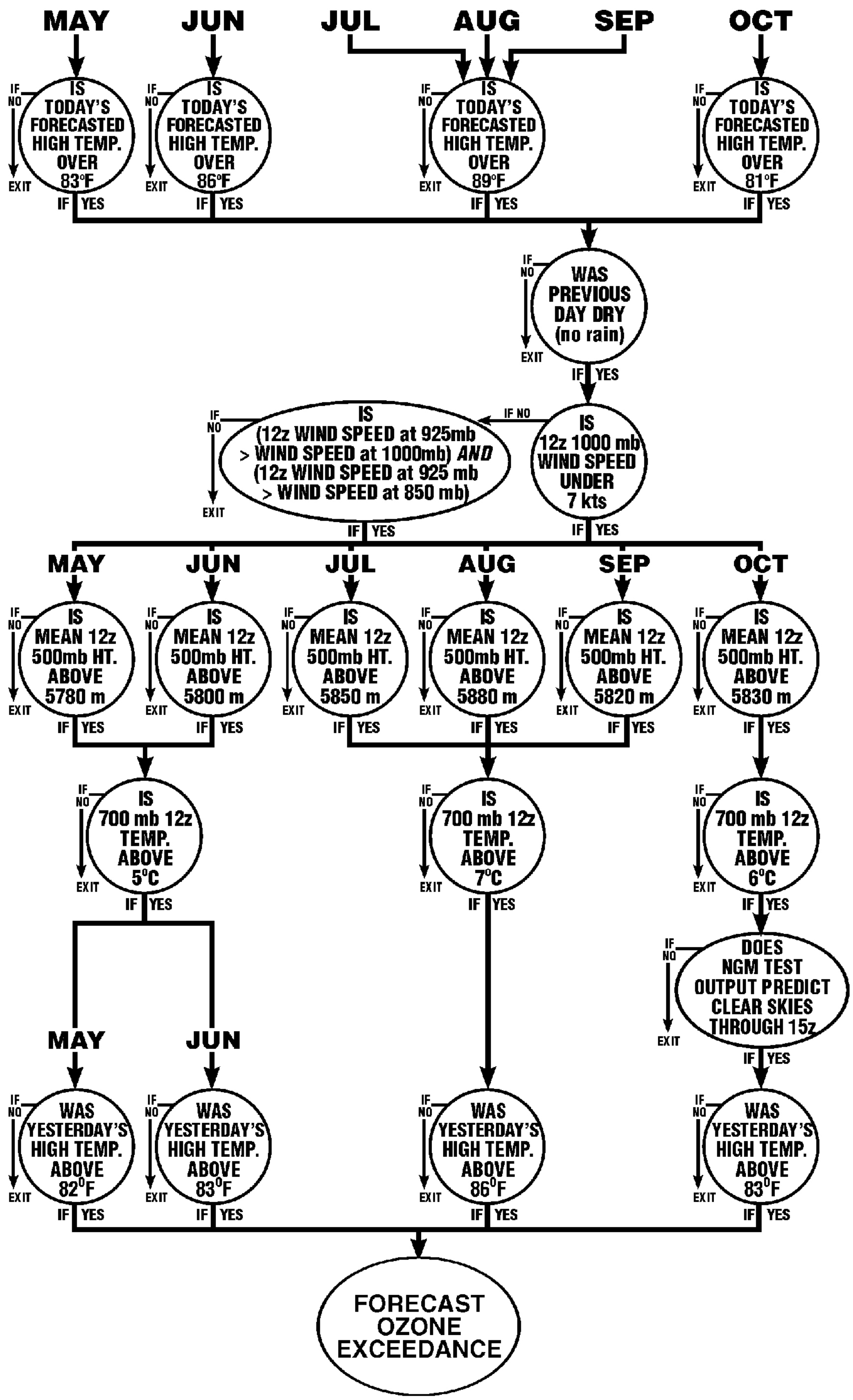

FIG. 4. Decision tree for nominal-scale forecasting of ozone exceedances at three or more sites in the Baton Rouge nonattainment zone.

warnings may have altered human activities and reduced the NO_x loadings on those days, thereby reducing the precursors and pollution below expected levels and causing some of these false positive forecasts to be made. Another important measure for binary variables is the threat score, which is similar to the probability of detection, but it offers the added benefit of penalizing both false alarms and missed occurrences, rather than only the missed occurrences (Aguado and Burt 2001). Thus, the probability of detection is an inflated measure of the model accuracy. Threat score is computed as the number of events forecast correctly divided by the sum

TABLE 8. Accuracy assessment of revised decision-making tree.

Forecast exceedance?	Actual exceedance?		
	Yes	No	Total
Yes	14	20	34
No	7	112	119
Total	21	132	153

of the total forecast events and the total actual events observed less the total of exceedance events correctly forecast. Thus, the threat score in the tree is given as 14/(34 + 21 − 14), or 34.1%. This represents an improvement over the 21.5% offered without the previous day's (binary) rainfall variable and additional wind stipulation noted above. These latter two criteria seem to be relatively uncommon in most regression-based ozone concentration models. These results collectively suggest that the decision tree may provide a useful means of forecasting exceedances, and similar but more elaborate methods such as the correlation and regression tree approach (e.g., Rodionov et al. 2001) may provide even more success.

e. *Two-model system verification: Does joint use of both models improve forecasting ability?*

Because both models appear to be useful but also have shortcomings, improved forecasts may result from an optimized use of the two models in combination. To assess the performance of the forecast models when used simultaneously, both the tree and regression models were retested separately and in concert using available data (including maximum temperature forecasts for the day in question) from 1 May to 31 October 2000 (i.e., the ozone season). Of the 178 days tested using the regression model, a Brier score (Wilks 1995) of 0.730 occurred when using a threshold of 85 ppb to forecast an exceedance. The disappointing model fit for 2000 is likely to result from poor temperature forecasts during that anomalously dry summer. However, for cases in which the predicted value of 105 ppb was used as the threshold for forecasting an exceedance, the Brier score fell dramatically to 0.230. In a similar way, for the 177 days examined using the decision tree, a Brier score of 0.297 was observed. The best predictive success occurred when exceedance forecasts were made only when both a regression-based estimate of at least 105 ppb and the decision tree indicated that an exceedance should be forecast. For this set of criteria, the Brier score fell to 0.158.

4. Summary and conclusions

A multiple-regression model, in combination with principal components analysis, was used to predict the 8-h peak ozone concentration at each site. The variables having the strongest PCA loadings along with afternoon temperature forecasts and previous day's maximum temperature were included in the multiple-regression model for each site. At individual stations, multiple-regression equations unfortunately failed to explain a high percentage of the dataset variance, possibly because of the potential local anomalous effects. The proximity of Baton Rouge to industrial sites to the south makes forecasting ozone inherently challenging, but the results also suggest that the region provides an ideal case study to investigate the local influence of NO_x transport into cleaner air. Further analysis revealed that a much better fit to the model can be found when the assumption that three site exceedances or more constitute a meteorologically predictable day. An appropriate equation for such analysis was provided.

Because of the difficulties of implementing and drawing conclusions from the quantitative models, a qualitative decision tree for forecasting ozone exceedance days under the proposed standard at three or more stations was constructed. The decision tree requires only readily available meteorological data at BTR for input. Despite having only a limited number of cases with which to test the model, results suggest that the decision tree may be a useful supplement to regression-based methods.

Based on the results of the two models, some generalizations can be stated about atmospheric and environmental conditions that favor high ozone concentrations in the Baton Rouge nonattainment zone. In general, to have a meteorologically favorable situation for producing exceedances at three or more stations on a given day, morning conditions should be cooler and drier than normal, winds should be lighter than normal, afternoon temperatures generally should be higher than normal, 0700 LST NO_x concentrations in the region should be high, cloud cover should be minimal, and no measurable rainfall on the previous day should have been reported. The combined use of the two models may provide improved forecasting of ozone exceedance days. Local NO_x variability and forecast afternoon maximum temperatures seem to be especially important factors in determining the ozone concentrations and in accuracy of prediction.

In future research, neural-network (e.g., Comrie 1997; Spellman 1999), artificial-intelligence/expert systems (Rodionov and Martin 1999), and correlation/regression-tree approaches (Rodionov et al. 2001) should be investigated to determine whether quantitative model performance may be improved through such techniques. In addition, time series techniques that can simulate the role of persistence of ozone concentrations may improve performance as well (RHB). Last, other meteorological contributions to tropospheric ozone in this region should be investigated, particularly tropopause-folding events (e.g., Reiter 1975; Varotsos et al. 1994; Tsutsumi and Makino 1995; Ravetta et al. 1999). Improved scientific understanding and forecasting techniques will allow for improved environmental planning efforts and both economic and aesthetic benefits.

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