REFINEMENT AND VALIDATION OF AN URBAN METEOROLOGICAL-POLLUTANT MODEL



Environmental Sciences Research Laboratory
Office of Research and Development
U.S. Environmental Protection Agency
Research Triangle Park, North Carolina 27711

RESEARCH REPORTING SERIES

Research reports of the Office of Research and Development, U.S. Environmental Protection Agency, have been grouped into five series. These five broad categories were established to facilitate further development and application of environmental technology. Elimination of traditional grouping was consciously planned to foster technology transfer and a maximum interface in related fields. The five series are:

- 1. Environmental Health Effects Research
- 2. Environmental Protection Technology
- 3. Ecological Research
- 4. Environmental Monitoring
- 5. Socioeconomic Environmental Studies

This report has been assigned to the ENVIRONMENTAL MONITORING series. This series describes research conducted to develop new or improved methods and instrumentation for the identification and quantification of environmental pollutants at the lowest conceivably significant concentrations. It also includes studies to determine the ambient concentrations of pollutants in the environment and/or the variance of pollutants as a function of time or meteorological factors.

This document is available to the public through the National Technical Information Service. Springfield, Virginia 22161.

REFINEMENT AND VALIDATION OF AN URBAN METEOROLOGICAL-POLLUTANT MODEL

by

Joseph P. Pandolfo Clifford A. Jacobs Robert J. Ball Marshall A. Atwater Joseph A. Sekorski

THE CENTER FOR THE ENVIRONMENT AND MAN, INC. Hartford, Connecticut 06120

68-02-1767

Project Officer

Jason Ching

Meteorology and Assessment Division Environmental Sciences Research Laboratory Research Triangle Park, N.C. 27711

Environmental Sciences Research Laboratory
Office of Research and Development
U.S. ENVIRONMENTAL PROTECTION AGENCY
Research Triangle Park, N.C. 27711

DISCLAIMER

This report has been reviewed by the Environmental Sciences Research Laboratory, U.S. Environmental Protection Agency, and approved for publication. Approval does not signify that the contents necessarily reflect the views and policies of the U.S. Environmental Protection Agency, nor does mention of trade names or commercial products constitute endorsement or recommendation for use.

FORWARD

Understanding of the phenomena and processes forming the reciprocal relationships between man and his environment has become essential. The Center for the Environment and Man, Inc. investigates these relationships in programs which are concerned with

- quantitative analysis and simulation of the physical characteristics of atmospheric and oceanic systems on all scales of action;
- the development and application of tools for the optimum use of environmental resources for mankind.

In this report, both major activities of the Center are reflected. It is concerned with the refinement and validation of a unique computer model which simulates the joint development of natural meteorological-oceanic systems and anthropogenic pollutant fields on the spatial scales of a major metropolitan region. The model can serve both as a research tool for the quantitative study of such systems, and as a component of future air quality management procedures.

F. C. Henriques Chief Executive Officer The Center for the Environment and Man, Inc.

ABSTRACT

New urban meteorological-pollutant model forecasts for the case described in Pandolfo and Jacobs (1973) were obtained and validated by the evaluation method proposed by Nappo (1974). Three new forecasts are described. The first retains the coarse (8 mile) horizontal resolution of the source emissions inventory previously used, but incorporates improved meteorological and pollutant input data. The second is like the first, but defines the source emissions inventory with finer (2 mile) horizontal resolution. The third is like the second, but incorporates increased vertical resolution below the prevalent inversion base level.

It is noted that the model should be credited with the production of a meteorological forecast as well as a pollutant forecast, in contrast to the others surveyed by Nappo. Most of these other models must be provided with a meteorological forecast as input. The evaluation statistics for the pollutant forecast by this model indicate that its meteorological forecast can be expected to be well suited as input to any pollutant forecast model.

Contrary to Nappo's suggestion, and our expectation, the evaluation statistics show that increasing the degree of horizontal detail of the source emission inventory did not, in this case, significantly increase the sensitivity and accuracy of the pollutant concentration forecast. In conformance with Nappo's previous finding, however, was the result that the detail of the vertical diffusion calculations was not very significant in determining the accuracy of the pollutant forecast. The validation statistics also indicate that making fuller use of the original capabilities of the model did significantly increase the accuracy of the forecast.

The results of the first ("new coarse") forecast prepared for this report show that the model is the least expensive of those surveyed by Nappo to run (except for the "persistence" model) when not charged with the cost of the meteorological prediction. This pollutant forecast is among the most accurate of those surveyed in terms of Nappo's overall average concentration and temporal correlation statistics. It is approximately accurate as other primitive equation models surveyed in terms of Nappo's standard error and spatial correlation statistics.

Because of these results, it is recommended that:

• the model described here be applied to generate meteorological predictions for input to more accurate pollutant forecast models where greater accuracy in spatial detail at smaller than metropolitan scale is desired.

- the model described here be applied as a pollutant forecast model where less accuracy in spatial detail is acceptable in return for low implementation costs; and
- a more accurate (higher order) computational scheme for the horizontal advection calculations be incorporated in the model. The development effort required to do this is relatively small, and the accuracy of spatial detail on the intra-metropolitan space scales could well be significantly enhanced.

This report was submitted in fulfillment of Contract No. 68-02-1767 by The Center for the Environment and Man, Inc. under the sponsorship of the U.S. Environmental Protection Agency. This report covers a period from February 1974 to November 1976, and the work was completed as of March 1976.

CONTENTS

Foreward	d	i.
Abstract	t	v
Tables .		i
Figures		.i
1.	Introduction	1
2.	The Planetary Boundary Layer Model	4
3.	The Input Data for This Experiment	5 .
	3.1 The modeled region	5
	3.2 Initial Fields	7
	3.3 Modifications of the thermal radiation by	
	atmospheric pollutants	8
4.	The Results of the Experiments	9
	4.1 Time series presentations	9
	4.2 Verification in terms of Nappo's statistics 1	.2
5.	Summary and Conclusions	.9
Referenc	ces	21
Technica	al Report Data Form	22
	•	
	TABLES	
Number	<u>Pa</u>	ıge
1	Model Evaluation Based on Temporal Characteristics	.3
2	Summary of Statistics for "New Forecasts"	.8

FIGURES

Number		Page
1	Basic equations used by the model	4
2	Locations of the horizontal grid used by Roth, et al. (1971) and the smaller area grid (fine and coarse) used in this	
. •	experiment	5
3	Heights (depths) of vertical grid levels in meters	6
4	Initial vertical temperature profiles used in forecasts	. 7
5-14	Time series of observed and forecast pollutant concentrations at measurement sites.	
	5 Reseda	9 9 10 10 10 11 11 11 11
15	Spatial distribution of temporal correlation coefficients R(t) for the "fine (horizontal) grid" and "new coarse (horizontal) grid" forecasts	. 14
16	$\overline{R(t)}^S$ versus $\overline{R(s)}^t$ average result for each model tested	15
17	Temporal variation of spatial correlation coefficients $R(s)$	16
18	$\overline{\sigma(t)}^{S}$ versus $\overline{\sigma(s)}^{t}$ average result for each model tested	17
19	Average and spread of temporal and spatial ratios	17

SECTION 1

INTRODUCTION

Nappo's (1974) survey indicated that a model previously developed at The Center for the Environment and Man, Inc. (CEM) under the Environmental Protection Agency (EPA) sponsorship (Contracts CPA 70-62 and 68-02-0223) and described in a report to EPA (Pandolfo, et al., 1973, EPA-R4-73-024a,b), produced pollutant forecasts with some verification statistics as accurate as those produced by more complex models, and at costs commensurate with simpler models. Nappo's analysis suggested again that a major source of inaccuracy (as measured by other verification statistics) was one proposed in that report--viz., the coarseness of the horizontal resolution of the model.

The abstract of that report follows:

The urban boundary-layer model, described in a previous report (Pandolfo, et al., 1972), was modified and used in forty test runs. Many of the runs varied the meteorological input about a standard (observed) set. It has, therefore, been demonstrated that an economical, objective, physically consistent, and precisely specified (though with some arbitrary elements) procedure has been achieved for obtaining and predicting the three-dimensional meteorological fields needed. In several of the runs, the input topography, landwater distribution, and other physical characteristics of the underlying surface were varied. The results demonstrate that ready generalization to other regions can be expected.

The modeled region was simulated with relatively coarse (8-mile) grid spacing. This is in contrast to other models which deal with pollutants only, and which are based on two-mile grid spacing (Sklarew, et al., 1971; Roth, et al., 1971). Nonetheless, the temporal and spatial variations of air temperature, humidity, and wind are simulated with an encouraging degree of realism. Temporal and spatial variations of CO are also simulated fairly realistically, with somewhat less accuracy than in the model described by Roth, et al. (1971), and with accuracy equivalent to that shown by Sklarew, et al. (1971). It is reasonable to expect improved simulation accuracy with the finer horizontal resolution used in these other models, and the performance of such simulations with this model is strongly urged.

Nappo's (1974) results formed the basis of a proposed scope of work for this project, which is defined as follows. This project was limited, as was the previous project, to the consideration of carbon monoxide (CO) as the subject pollutant. Therefore, no attempt was made to model chemical changes. It was further proposed that:

- The model described in the EPA report (EPA R4-73-025a,b) be modified to allow 2-mile square resolution in the CO prediction and CO input source distribution, with no other changes.
- A single test prediction be run for the case previously treated (Los Angeles, 14GMT, 29 September 1969 through 04GMT, 30 September 1969).
- The accuracy of this pollution prediction be evaluated and compared to that of other pollution models using the method of Nappo (1974).
- The computer costs for the prediction be fully documented.
- A summary report, supplementing our previous report, be submitted on the results of this single experiment.

As proposed, this scope of work would have resulted in an experiment in which two pollutant forecasts would have been compared—those resulting from a "coarse (horizontal) grid" model, and those resulting from a "fine (horizontal) grid" model. During the course of the work, it was decided, with the agreement of the contract monitor, to expand the scope of the work, at no additional cost to the sponsor, to take advantage of several capabilities of the coarse (horizontal) grid model which had not been previously used, and to obtain forecasts with

- greater vertical resolution below the prevalent temperature inversion base level (at about 150m in height) and coarser vertical resolution above this level;
- 2) initial vertical profiles of temperature in the soil and lower atmospheric layer over the modeled region whose local shapes were generated by the 24-hour forecasts previously obtained with the model; but whose absolute values were determined by the initial sparse set of temperature observations available from the five weather stations in the region;
- 3) calculated absorption/scattering of solar and radiation by NO₂ and particulates; NO₂ and particulate concentrations used in these calculations were assumed to be fixed fractions of the predicted CO concentration at any given place and time.

The scope was additionally expanded through the use of hourly averages of model-predicted pollutants in the validation, rather than the single-time step values previously used (the observations are hourly averages). Also, changes in several of the initial pollutant concentrations were made to provide better agreement with the observed values at the initial time and at nearby stations.

This expansion of scope now allowed three forecasts to be compared; viz.

- the "old coarse (horizontal) grid" forecast previously validated in Pandolfo, et al. (1973), and Nappo (1974);
- a "new coarse (horizontal) grid" forecast; and
- a "fine (horizontal) grid" forecast.

Improvements in accuracy of the second forecast over the first can thus be attributed to fuller use of the meteorological capabilities of the original model and in the changes made in the initial concentrations. Improvements on accuracy of the third forecast over the second can be attributed to refinement of the horizontal resolution of the source emission fields and pollutant predictions.

Finally, we refined the vertical grid still further to approximate the vertical resolution used by Roth, et al. (1971), and obtained another set of new forecasts. These "fine vertical grid new forecasts" did not exhibit better verifications than the other "new" forecasts as will be shown later.

SECTION 2

THE PLANETARY BOUNDARY LAYER MODEL

The model equations remain as outlined in Section 2.0 and Appendix C of Pandolfo and Jacobs (1973).

The only changes to the model are those which allow the optional use of a finer horizontal grid for the solution of the conservation equation for one of the pollutants, than that used in the solution of the conservation equations for all other variables. The program, as described in an addendum to this report, now allows the finer grid to have a grid length which is an integral fraction $[I]^{-1}$ of the basic meteorological grid length, where I can range from 1 to 4.

A summary of the modeling equations is also included here for handy reference (see Figure 1).

FORM
$$\frac{\partial x_{i}}{\partial t} + \overrightarrow{V} \cdot \nabla x_{i} = \frac{\partial}{\partial z} \left[K_{i} \frac{\partial x_{i}}{\partial z} \right] + A_{i}$$

ATMOSPHERE
$$\frac{\partial u}{\partial t} = -\overrightarrow{V} \cdot \nabla u + \frac{\partial}{\partial z} \left[K_{m} \left(R_{i}, z \right) \frac{\partial u}{\partial z} \right] + t \left[v - v_{g} \right]$$

$$\frac{\partial y}{\partial t} = -\overrightarrow{V} \cdot \nabla v + \frac{\partial}{\partial z} \left[K_{m} \left(R_{i}, z \right) \frac{\partial v}{\partial z} \right] - t \left[u - u_{g} \right]$$

$$\frac{\partial T}{\partial t} = -\overrightarrow{V} \cdot \nabla t + \frac{\partial}{\partial z} \left[K_{\theta} \left(R_{i}, z \right) \frac{\partial T}{\partial z} \right] + \Gamma \frac{\partial K_{\theta}}{\partial z} + w\Gamma + \left(\frac{\partial T}{\partial t} \right)_{rad}$$

$$\frac{\partial u}{\partial t} = -\overrightarrow{V} \cdot \nabla u + \frac{\partial}{\partial z} \left[K_{\theta} \left(R_{i}, z \right) \frac{\partial u}{\partial z} \right] + S_{p}$$

$$\frac{\partial u}{\partial t} = -\overrightarrow{V} \cdot \nabla u + \frac{\partial}{\partial z} \left[K_{\theta} \left(R_{i}, z \right) \frac{\partial u}{\partial z} \right] + S_{p}$$
SOIL
$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left[K_{s} \left(z \right) \frac{\partial T}{\partial z} \right]$$
INTERFACE ENERGY BALANCE
$$0 = R_{s} \left(1 - a \right) + R_{a} - \sigma T_{1}^{4} - LE - A - S + R_{m}$$

Figure 1. Basic equations used by the model.

SECTION 3

THE INPUT DATA FOR THIS EXPERIMENT

3.1 THE MODELED REGION

The specification of the modeled region remains as defined in Section 3.1.1 of Pandolfo, et al. (1973), with the following exceptions.

The fine horizontal grid cell dimension of 2 miles is specified for the pollutant, along with the coarser 8-mile grid dimension used for the other variables. The two grid arrays, and their location in the Los Angeles region are shown in Figure 2.

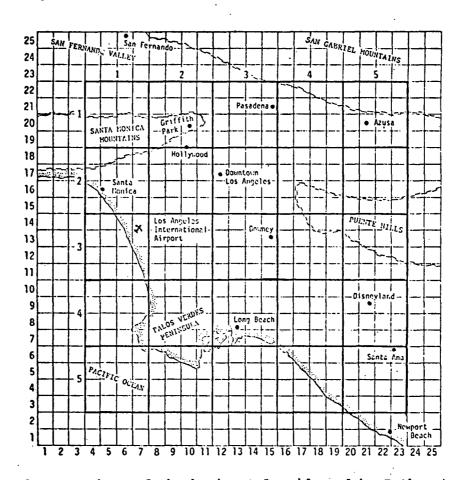


Figure 2. Locations of the horizontal grid used by Roth, et al. (1971) and the smaller area grid (fine and coarse) used in this experiment.

The vertical layer modeled extends, as previously, from 200m below the air-soil(water) interface to 1500m above this interface. However, the grid levels used in the new forecasts have been changed as described in Section 1 of this report. The old set and the new set of vertical grid levels are shown in Figure 3. The "finer vertical" set of vertical grid levels is also shown.

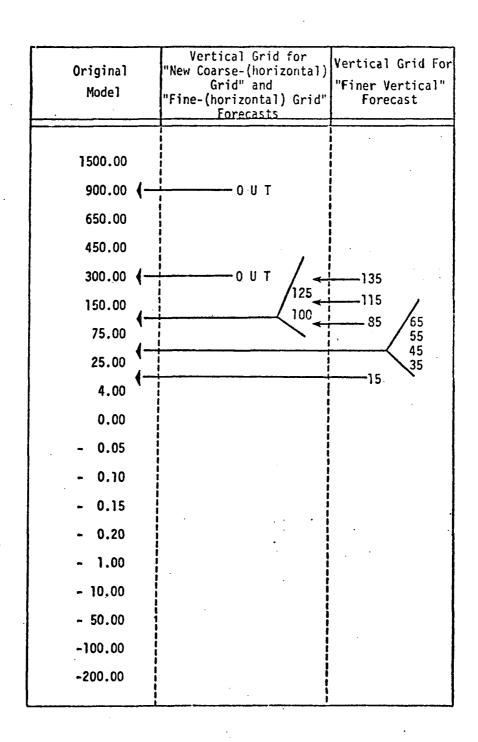


Figure 3. Heights (depths) of vertical grid levels in meters.

3.2 INITIAL FIELDS

The initial fields of the variables specified in Section 3.1.3 of Pandolfo, et al. (1973) were used with the temperature and pollutant fields modified as described in Section 1 above. A comparison of the originally used and modified initial vertical profiles of temperature at the center of the modeled regions is shown in Figure 4.

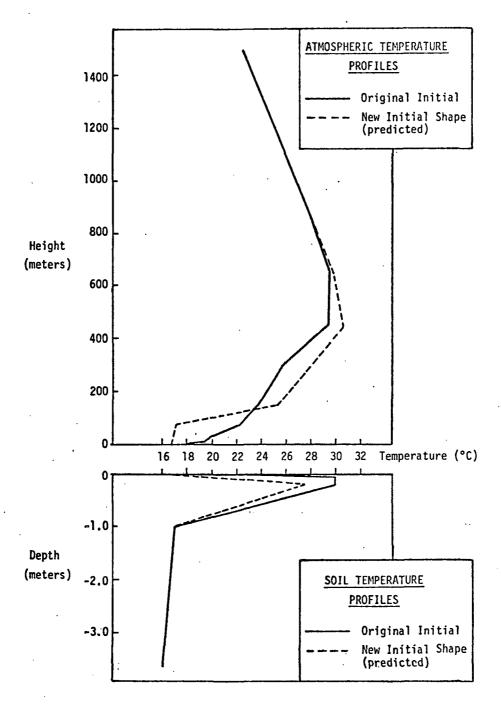


Figure 4. Initial vertical temperature profiles used in forecasts.

3.3 MODIFICATION OF THE THERMAL RADIATION BY ATMOSPHERIC POLLUTANTS

The original model had the potential for including in the meteorological forecast the radiative effects of selected pollutants. In its most complete form, the model would include each of two radiatively active pollutants as separate dependent variables whose concentrations are to be predicted. Atwater's (1971) work, based on a simplified version of this model, had, however, identified the nitrogen oxide (NO₂) and the particulate aerosols as the only constituents with significant radiative effects. In the present experiment, the inclusion of these radiative pollutants was, therefore, carried out in a much simpler manner than that originally developed. We first assumed that the concentrations of the radiatively active pollutants could be represented as fixed fractions of the CO, whose concentration was explicitly predicted. This assumption was justified by analysis of the observed concentrations which were available for study,* and which established concentration ratios.

These concentration ratios were then combined with actual values of the solar absorption coefficient for NO_2 , the solar absorption, solar scattering, and infrared absorption coefficients for aerosol particulates to obtain a corresponding set of "fictitious" radiative coefficients for the only pollutant that was explicitly predicted--viz., the CO. These "fictitious" coefficients, valid for 1 ppm NO_2 and urban particulate aerosols, are:

- solar absorption coefficient = .15 km
- solar scattering coefficient = .15 km⁻¹
- infrared absorption coefficient = 0 km⁻¹
- infrared scattering coefficient = 0 km⁻¹

These coefficients are used with the simulated CO concentrations and the concentration ratios to compute the actual coefficient at each time step.

^{*} Obtained from the Los Angeles Air Pollution Control District.

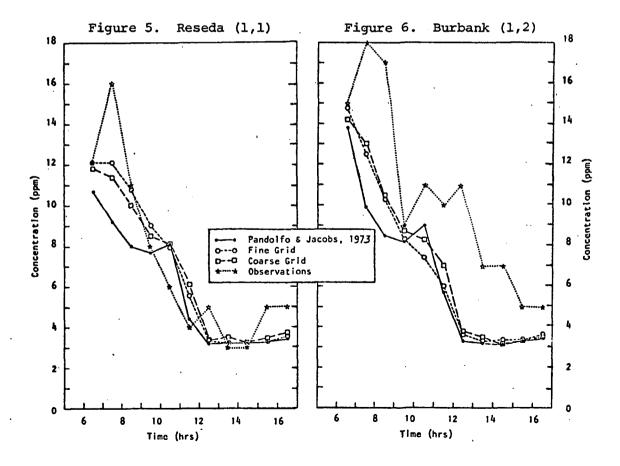
SECTION 4

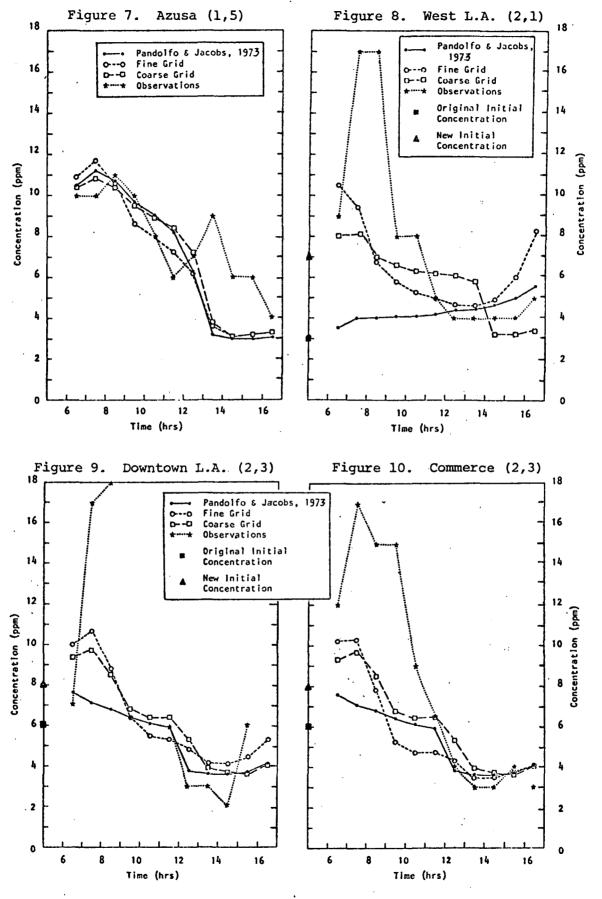
THE RESULTS OF THE EXPERIMENTS

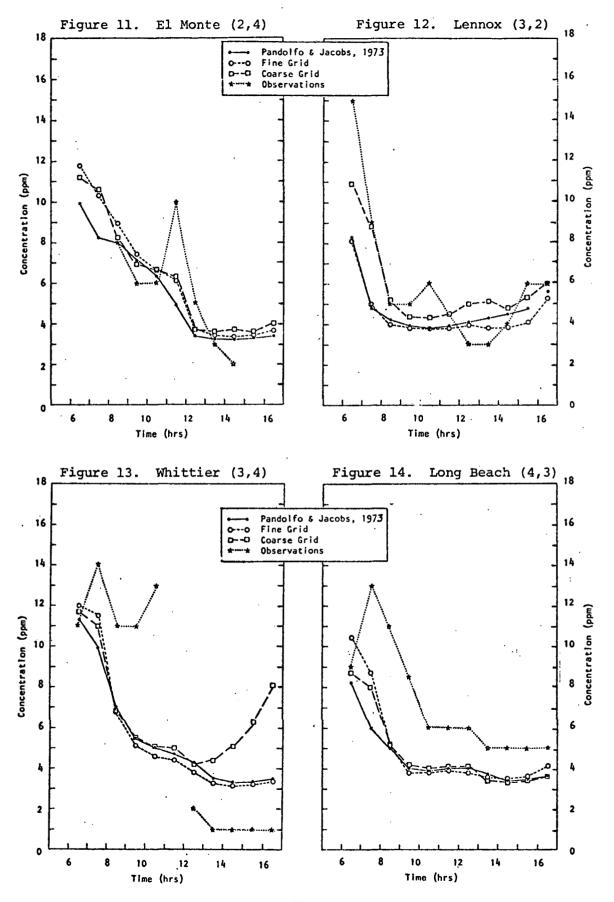
4.1 TIME SERIES PRESENTATIONS

Time series of predicted CO concentrations at the 4-m grid level, at each of the measuring stations are shown in Figures 5 through 14. Also shown are the measured values, and the values previously reported and validated from the "old coarse (horizontal) grid" forecasts (Pandolfo, et al., 1973; Nappo, 1974). Two "new" forecasts are shown--one for the "fine (horizontal) grid" and one for the "new coarse (horizontal) grid."

Figures 5 through 14. Time series of observed and forecast pollutant concentrations at measurement sites.







While it is difficult to summarize the comparative results from this presentation, some qualitative features are evident. First is that the "new" forecasts are slightly more realistic than the "old" forecasts. Second is that only slight differences between the "new coarse (horizontal) grid" forecast and the "fine (horizontal) grid" forecast are evident.

One change in the validation procedure should be noted. In the "old" forecasts, "instantaneous" (4.8 minute average) predicted values on the hour were compared with hourly average observed values centered on the half hour. In the "new" forecasts, hourly average predicted values centered on the half hour are used in the verification. Some of the improvement noted in the statistical verifications of the "new" forecasts that follow may be attributed to this change.

4.2 VERIFICATION IN TERMS OF NAPPO'S STATISTICS

The statistics suggested by Nappo in his 1974 paper for the evaluation of pollutant predictions are

- the spatial average of temporal correlation coefficient, R(t)s;
- the temporal average of the spatial correlation coefficient, $R(s)^{t}$;
- a "spread", or temporal average of standard deviation of the radios of predicted-to-observed map values at a given time, $\overline{\sigma(s)}^t$;
- a "spread" or spatial average of standard deviation of the ratios of predicted to observed time series values at a given place, $\sigma(t)^s$,
- the spatial average of the ratios of predicted-to-observed values as seen in time series at a given place, $r(t)^s$;
- the temporal average of the ratios of predicted-to-observed values as seen on maps at given times, $r(s)^t$.

Nappo showed that, when a validation sample was distributed in both space and time, the last two statistics were identical; i.e.,

$$\overline{r(t)}^{s} = \overline{r(s)}^{t}$$
.

The graphs presented in this section are those of Nappo, with points added for the two new forecasts obtained in this project, which are identified as "Pandolfo, et al. (1976)".

We first reproduce Nappo's summary table of temporal characteristics (Table 1) with the newly validated forecast summaries added. The station-to-station variation of R(t) is shown in Figure 15. In Table 1, we show the spatial average $R(t)^S$.

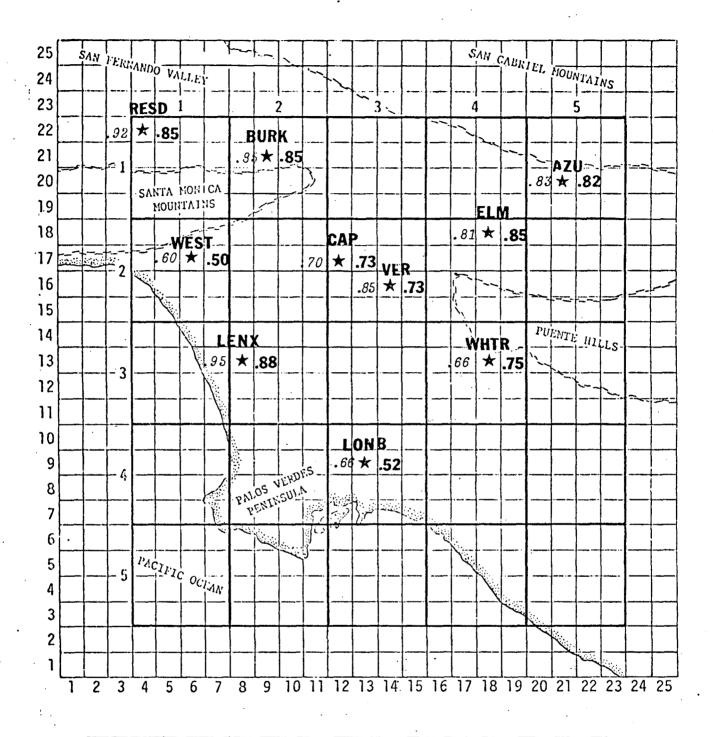
TABLE 1

MODEL EVALUATION BASED ON TEMPORAL CHARACTERISTICS

MODEL	Average Temporal Correlation Coefficient	IBM 360/65 Computer Time for 24-hour Prediction (minutes)	Computer Cost for 24-hour Prediction (dollars)
MacCracken, et al. (1971) multi-box	0.37	106	350
24-Hour Persistence	0.47	none	none
Roth, et al. (1971) primitive equation	0.52	60	200
Hanna (1973) ATDL simple model	0.60	none	none
Sklarew, et al. (1972) particle-in-cell	0.65	49	160
Pandolfo and Jacobs (1973) primitive equation ("Old coarse (horizontal) grid" forecast)	0.66	20	70
Reynolds, et al. (1973) primitive equation	0.73	30	100
Eschenroeder, et al. (1972) trajectory	0.73	. 15	50
Lamb and Neiburger (1971) trajectory	0.90	35	115
Pandolfo, et al. (1976) primitive equation	·.		×1.
Coarse (horizontal) Grid Fine (horizontal) Grid Finer Vertical, Fine (horizontal) Grid	0.75 0.79 0.80	18 * 144 * 150 *	60 † 480 † 500 †

^{*} Converted from CDC 7600 running time using the ratio 25 min (IBM 360/65) = 1 min (CDC 7600).

[†] Estimated at Nappo's average of \$3.33/min (IBM 360/65). Actual costs experienced in this project on CDC 7600 @ \$2580/hour were slightly lower than these.



WEY: "Fine" indicated in italics at the left of the measuring site.
"New Coarse" indicated in bold numbers at the right of the measuring site.

Figure 15. Spatial distribution of temporal correlation coefficients R(t) for the "fine (horizontal) grid" and "new coarse (horizontal) grid" forecasts.

Figure 16 shows $R(t)^S$ and $R(s)^t$ for the models evaluated by Nappo, with the two forecasts made in this project added. The best result that a forecast could achieve would fall at the coordinates 1,1 in this figure.

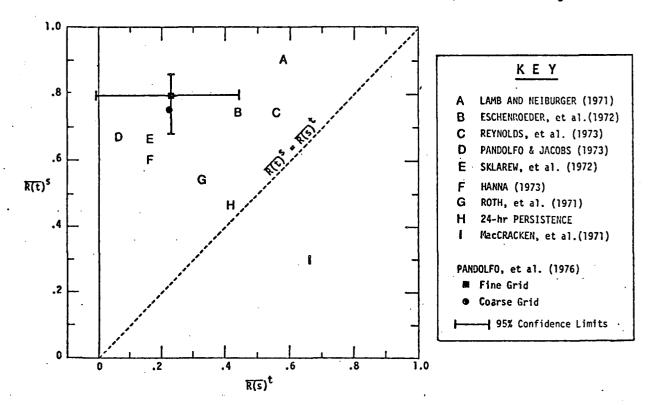


Figure 16. $R(t)^{S}$ versus $R(s)^{t}$ average result for each model tested.

Also added to Figure 16 are the 95 percent confidence limits obtained by using Fisher's (1925) transformation for the correlation coefficient, which allows the confidence limits to be evaluated for an aggregate of several correlation coefficients, each obtained from a sample with a small number of pairs. These confidence limits add greater perspective to the significance of the statistics, $R(t)^S$ and $R(s)^t$, with the sample sizes available for Nappo's validation study.

From Figure 16 it appears that no significant improvement in these statistics was obtained by going from the "new coarse (horizontal) grid" forecast to the "fine (horizontal) grid" forecast at a large increase in cost. However, a barely (at the 95% level) significant improvement was obtained by the "new coarse" forecast over the "old coarse" forecast at no increase in cost.

The hour-to-hour variations of the spatial correlation coefficient R(s) are shown in Figure 17. An interesting feature of these variations is that more skill is attained in the two forecasts tabulated here, for those hours in which relatively high levels of CO concentration are present--viz., the morning peak hours (see Figures 5-14) between 0630 and 0930 and the onset of the evening peak at the last hour of observations (viz., 1630). The lack of skill in spatial prediction is confined to the hours between 1030 and 1530,

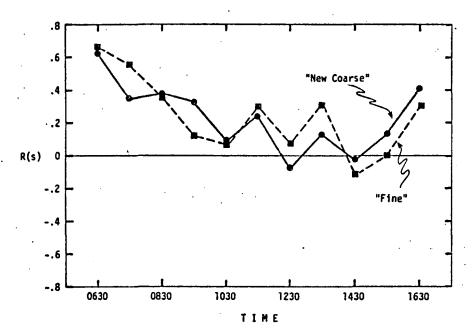


Figure 17. Temporal variation of spatial correlation coefficients R(s) .

during which background levels of 3 to 5 ppm are prevalent. This could be a feature common to all the primitive equation models evaluated by Nappo, and, if so, the apparent advantage of the other types of model in obtaining higher temporal averages of the spatial correlations would be of little operational significance.

The "spreads" or average standard deviations $\sigma(s)^{t}$ and $\sigma(t)^{s}$ of the ratios (predicted-to-observed) are shown in Figure 18. The best result that could be achieved by a model would fall at the origin of this graph. Again, no significant improvement is achieved in going from the "new coarse (horizontal) grid" forecast to the "fine (horizontal grid" forecast in a large additional cost. Significant improvement is obtained in going from the "old coarse (horizontal) grid" forecast to the "new coarse (horizontal) grid' forecast at no additional cost.

The "spreads" and average values of the ratios are plotted on Figure 19. The best result that could be achieved by a forecast would be represented by a point falling at 1,1 with zero spread in both coordinate directions. Here the differences between the "new coarse (horizontal) grid" and "fine (horizontal) grid" forecasts are so small that only one is plotted. These forecasts did not improve the average ratio (predicted-to-observed) score obtained by the "old coarse (horizontal) grid" forecast, which was the best of all the models surveyed by Nappo.

The values of each of the statistics obtained in the two forecasts are summarized in Table 2. Also shown in this table are the statistics obtained in the "finer vertical grid, fine (horizontal) grid" forecast.

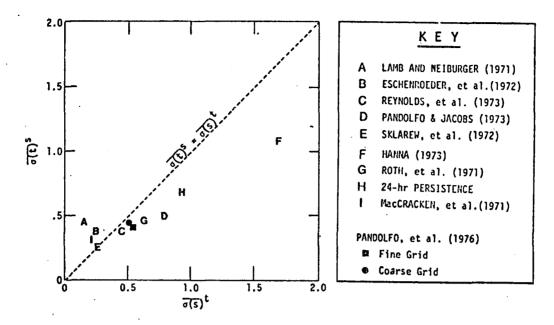


Figure 18. $\overline{\sigma(t)}^s$ versus $\overline{\sigma(s)}^t$ average result for each model tested.

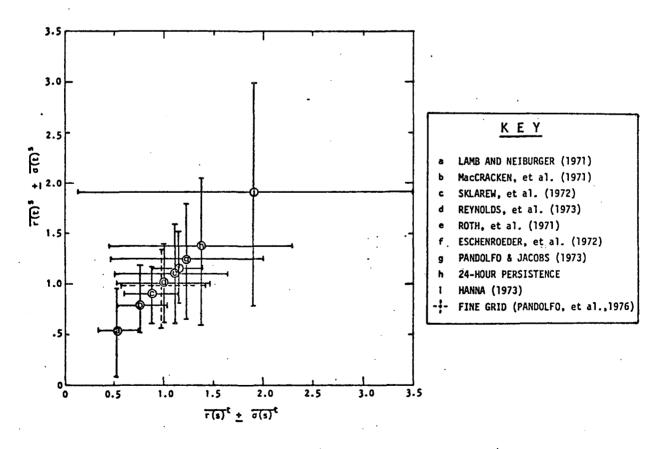


Figure 19. Average and spread of temporal and spatial ratios.

TABLE 2
SUMMARY OF STATISTICS FOR "NEW FORECASTS"

GRID	R(t) ^s	R(s) t	σ(t) ^s	σ(s) ^t	$\overline{r(t)}^{S} = \overline{r(s)}^{t}$
New coarse (horizontal)	.75	.23	.42	.50	1.02
Fine (horizontal)	.79	.24	.41	.52	1.04
Finer vertical, Fine (horizontal)	.80	.20	.37	.44	. 98

SECTION .5

SUMMARY AND CONCLUSIONS

In comparing the costs incurred by the models he surveyed (see Table 1 of this report), Nappo ignored the fact that the cost of running the Pandolfo and Jacobs (1973) model included the generation of four-dimensional (x,y,z,t) fields of wind, temperature, and diffusivity. None of the other models surveyed were charged with the presumably greater costs of subjectively and laboriously prespecifying these fields on a case-by-case from a sparse set of raw meteorological observations. About half the computer costs ($\sim \$30/24$ -hour prediction) of the coarse (horizontal) grid models described in this report are attributable to the thermal radiation calculations alone. Of the remaining half of the computer costs, about one-sixth is attributable to the CO prediction (this gross upper limit is obtained by assuming that the remainder of the primitive equation prediction of u , v , T_{air} , q , $T_{soil}T_{water}$, and CO can be equally apportioned). This means that the coarse (horizontal grid CO predictions should, at most, be charged with \$5/24-hour prediction for a valid comparison of costs with the other models, except the "persistence" model.

The correct way to look at this factor is, however, the reverse. That is, the primitive equation model described in this report generates the necessary meteorological data in the appropriate form for something under \$60/24-hr prediction. All of the other models (except the "persistence" model) require, before they can be applied, the specification of spatially and/or temporally varying fields of at least wind and inversion height for each day and region.

These would have to be obtained with only about four man-hours of a \$15,000 per year meteorologist, assuming a \$15,000/year overhead load, or the equivalent in additional computer costs, for our costs to be equal. Therefore, it would be fairer to add about \$60/24-hr prediction to Nappo's tabulated costs (Table 1) for all models other than those described here, except the "persistence" model.

This having been said, the first conclusion to be stated is one that is contrary to Nappo's suggestion and to our expectation, in the case of the model used in this study. Table 2 shows that increasing the degree of detail of the source emissions inventory did not, in this case, significantly increase the sensitivity and accuracy of the pollutant concentration forecast. This result, in hindsight, can only be attributed to the fact that the calculation scheme used for the horizontal advection calculations—viz., the upwind—difference scheme—has an inherent degree of approximation that masks the increase in accuracy that might have been expected from treating the source emissions inventory in greater detail.

If we compare results for the "fine (horizontal) grid" and "finer vertical,

fine (horizontal) grid" forecasts in Table 2, however, we find that another of Nappo's findings is confirmed in this case. This is that "the detail of the vertical diffusion calculations is not very significant in determining a model's accuracy."

Comparison of the results for the "new coarse (horizontal) grid forecast" and the "Pandolfo-Jacobs (1973) forecast" shows that making fuller use of the inherent meteorological capabilities of the model used in these studies does significantly increase the accuracy of the forecast. These features were exploited by combining model-generated vertical profiles of temperature with observed surface temperatures to obtain initial temperature fields, and allowing radiatively active pollutants to affect the predicted temperatures at no significant increase in forecast cost.

Some of the improvement noted in the "new coarse (horizontal) grid" forecast results may also be attributed to the validation of predicted hourly averages instead of predicted single-time step concentrations as was done by Pandolfo and Jacobs (1973).

Finally, we restate some of the results presented in Table 1 and Figures 16, 18, and 19. These are that in the "coarse (horizontal) grid model" forecasts made here,

- the forecast is among the least expensive to run, and is, in fact, the least expensive to run when it is credited with the generation of the meteorological predictions needed by all the other models except the "persistence" model;
- the pollutant forecasts are among the most accurate in terms of Nappo's $R(t)^S$ and $r(s)^t$ statistics; and
- the pollutant forecasts are of about average accuracy in terms of Nappo's $R(s)^t$, $\sigma(s)^t$, and $\sigma(t)^s$ statistics.

The adequacy of the pollutant forecasts suggests that the meteorological predictions yielded by the model are well suited for input to any pollutant prediction model requiring such inputs--e.g., all the models surveyed by Nappo except the "persistence" model.

The results suggest that, in the near future

- the model described here be applied to generate meteorological predictions for input to more accurate pollutant forecast models where great accuracy in spatial detail at smaller than metropolitan region scales is desired;
- the model described here be applied as a pollutant forecast model where less accuracy in spatial detail is acceptable in return for low implementation costs; and
- a more accurate (higher order) computational scheme for the horizontal advection calculations be incorporated in the model. The development effort required to do this is relatively small, and the accuracy of spatial detail on the intra-metropolitan space scales could well be significantly enhanced.

REFERENCES

- Atwater, M.A., 1971: Radiation effects of pollutants in the atmospheric boundary layer. J. Atmos. Sci., 23, 1367-1373.
- Fisher, R.A., 1925: Statistical Methods for Research Workers, 1st Edition (12th Edition, 1954), Oliver and Boyd, Edinburgh.
- Nappo, C.J., Jr., 1974: A method for evaluating the accuracy of air pollution models. Preprints, Symposium on Atmospheric Diffusion and Air Pollution, Sept. 9-13, 1974, Santa Barbara, California, American Meteorological Society, Boston, Mass., 325-329.
- Pandolfo, J.P, M.A. Atwater, and G.E. Anderson, 1971: Prediction by Numerical Models of Transport and Diffusion in an Urban Boundary Layer, Final Report Vol. I, The Center for the Environment and Man, Inc., Hartford, Conn., 139 pp.
- ______, and C.A. Jacobs, 1973: Tests of an Urban Meteorological Pollutant Model
 Using CO Validation Data in the Los Angeles Metropolitan Area. Final Report EPA Contract No. 68-02-0223 (EPA-R4-73-025a), NERC, USEPA, Durham,
 N.C.
- Roth, P.M., S.D. Reynolds, P.J.W. Roberts, and J.H. Seinfeld, 1971: Development of a Simulation Model for Estimating Ground Level Concentrations of Photochemical Pollutants. Final Report, 71 SAI-21, Systems Applications, Inc., Beverly Hills, Calif., 51 pp., Appendices A-F.
- Sklarew, R.C., A.J. Fabrick, and J.E. Prager, 1971: A Particle-in-Cell Method for Numerical Solution of the Atmospheric Diffusion Equation, and Applications to Air Pollution Problems. Final Report, 3SR-844, Systems, Science, and Software, LaJolla, Calif., 163 pp.

TECHNICAL REPORT DATA (Please read Instructions on the reverse before completing)				
I. REPORT NO. EPA-600/4-76-037	2.	3. RECIPIENT'S ACCESSION NO.		
4. TITLE AND SUBTITLE REFINEMENT AND VALIDATION	5. REPORT DATE July 1976			
POLLUTANT MODEL.	6. PERFORMING ORGANIZATION CODE			
Joseph P. Pandolfo, Clifford A. Jacobs, Robert J. Ball, and Marshall A. Atwater		B. PERFORMING ORGANIZATION REPORT N		
P. PERFORMING ORGANIZATION NAME AND ADDRESS The Center for the Environment and Man, Inc.		10. PROGRAM ELEMENT NO.		
		1AA009		
275 Windsor Street	11. CONTRACT/GRANT NO			
Hartford, Connecticut 06				
	68-02-1767			
12. SPONSORING AGENCY NAME AND AL	13. TYPE OF REPORT AND PERIOD COVERED			
Environmental Sciences Re	Final Report 2/24 - 11/76			
Office of Research and Development		14. SPONSORING AGENCY CODE		
U.S. Environmental Protec				
Research Triangle Park, N	EPA-ORD			
5. SUPPLEMENTARY NOTES				

16, ABSTRACT

This report discusses the refinement of a grid point model for predicting atmospheric transport and diffusion in an urban boundary layer. In earlier studies, a coarse 8-mile horizontal square grid was used to predict CO concentrations in the Los Angeles Metropolitan area. In this study, a 2-mile grid for the CO emission has been used to test a recent hypothesis that predictive accuracy can be improved by incorporating a finer horizontal grid resolution to more accurately reflect the spatial distribution of a pollutant emission pattern. However, contrary to expectations, the evaluation statistics show that increasing the degree of horizontal detail in the source emission inventory did not significantly increase the sensitivity and accuracy of the pollutant concentration forecast.

When compared to other models, this pollutant forecast is among the most accurate when predicting the overall average concentration and temporal correlation, and approximately as accurate as other primitive equation models in terms of spatial correlation statistics.

17.	KEY WORDS AND DOCUMENT ANALYSIS				
).	DESCRIPTORS	b.identifiers/open ended terms	c. COSATI Field/Group		
*Air pollution *Meteorological data *Mathematical models *Atmospheric models *Models tests *Forecasting			13 B 04 B 12 A 04 A 14 B		
s. DISTRIBU	TION STATEMENT	19. SECURITY CLASS (This Report) UNCLASSIFIED	21. NO. OF PAGES		
RELEASE TO PUBLIC		20. SECURITY CLASS (This page) UNCLASSIFIED	22. PRICE		

EPA Form 2220-1 (9-73)