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MASTER

Development and Testing of an Air Quality Model for Mexico City

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INTRODUCTION

Los Alamos National Laboratory and Instituto Mexicano del Petroleo have embarked on a joint study of options for improving air quality in Mexico City. The intent is to develop a modeling system which can address the behavior of pollutants in the region so that options for improving Mexico City air quality can be properly evaluated. In February of 1991, the project conducted a field program which yielded a variety of data which is being used to evaluate and improve the models. Normally the worst air quality for both primary and photochemical pollutants occurs in the winter in Mexico City.

During the field program, measurements included: (1) lidar measurements of aerosol transport and dispersion, (2) aircraft measurements of winds, turbulence, and chemical species aloft, (3) aircraft measurements of earth surface skin temperatures, and (4) tethersonde measurements of wind, temperature and ozone vertical profiles.

The Mexico City Metropolitan Area (MCMA)lies at an elevation of approximately 7500 feet above sea level in a "U" shaped basin which opens to the north. Mountains on the east and southeast sides of the basin form a barrier with a height of approximately 12,000 feet while two isolated peaks reach elevations in excess of 17,000 feet. The city occupies a major part of the southwest portion of the basin. Upper level winds are provided by rawinsondes at the airport, low-level winds are measured at several sites within the city. Many of the sites have obstructed upwind fetches for a variety of directions.

A three-dimensional, prognostic, higher order turbulence meteorological model (HOTMAC) was modified to include an urban canopy and urban heat sources. HOTMAC is used to drive a Monte-Carlo kernel dispersion code (RAPTAD). HOTMAC also provides winds and mixing heights for the CIT photochemical model which was developed by investigators at the California Institute of Technology and Carnegie Mellon University.

THE METEOROLOGICAL MODELING SYSTEM

Model Formulation

HOTMAC is a three-dimensional time-dependent model developed by T. Yamada[1]. It uses the hydrostatic approximation and a terrain following coordinate system. HOTMAC solves conservation relations for the horizontal wind components, potential temperature, moisture, turbulent kinetic energy, and the turbulence length scale. HOTMAC describes advection, Coriolis effects turbulent transfer of heat, momentum, and moisture. It also describes solar and terrestrial radiation effects, turbulent history effects, and drag and radiation effects of forest canopies.

The development of the equations and form of the factors is described by Yamada[2] and Mellor and Yamada[3].

The lower boundary conditions are defined by a surface energy balance and similarity theory. The soil heat flux is obtained by solving a heat conduction equation in the soil which ignores lateral heat transfer. In an urban context the surface energy balance requires an additional term which represents the heat released by man's activities. The additional heat along with differences in thermal and albedo properties between urban and non-urban surfaces produces the urban heat island.

Meteorological Model Application

Early in the project, three days in which air quality was poor, good, and normal were chosen for detailed modeling. All of the days were in winter of 87-88. Meteorological inputs were based on the afternoon rawinsonde of the preceding days which was used to estimate synoptic scale wind and temperature profiles.

We used a nested grid system to model the valley of Mexico and its surrounding terrain. The outer grid has a 6 km spacing and covers the major terrain influences as shown in figure 1a. The inner grid as shown in figure 2a embraces the city and the immediately adjacent slopes. The individual characters plotted on the figure are monitoring sites operated by the Mexican Urban Development and Ecology Secretariat. The four character labels are sites used by the lidar. The inner grid has a size of 2 km. The urban canopy was approximated by using the estimated distribution of CO emissions defined on a 1 km grid. The relative CO emissions were used to proportion the fraction of the area of a grid cell which was covered by canopy (roof tops), the average soil conductivity, average soil heat capacity, and the urban heat release intensity. Many of the parameters used to represent the urban canopy are first estimates which will be refined as more information on land use and urban skin temperatures becomes available during the course of the study.

The modeling showed that the meteorology of the region could be reasonably represented by the modeling system on days with poor ventilation and consistent upper level winds. However, with changing upper level winds the model gave poor results. In the 1991 simulations the model was altered to nudge the winds at the one and two kilometer levels towards the available measurements. Another area in which model deficiencies were noted, related to the timing of the development of slope winds near the urban area. The early model results suggest that the urban heat island in the model is too strong so that the upslope winds are retarded in the morning while the downslope winds are advanced in the evening. This paper describes the modeling for a single period, Feb. 21 and 22 during which a typical high pollution day occurred. Work on other periods during the field program is not yet complete.

THE PARTICLE TRANSPORT CODE RAPTAD

Model Formulation

RAPTAD is a Monte Carlo random particle statistical diffusion code, developed by Ted Yamada[4]. Pseudo-particles are transported with instantaneous velocities that include the mean wind field and the turbulence velocities. The turbulence velocity is generated randomly consistent with the standard deviation of the wind at the particle location. The location of each pseudo-particle represents the center of mass of a concentration distribution for each puff. The total concentration at any point is obtained by adding the concentration contributions of each puff at that point (a kernel method).

The Monte Carlo kernel method requires that a functional form for the distribution kernel be chosen and that parameters that describe the width, breadth, and depth of the distribution be calculated. The approach used here is to assume a Gaussian distribution where variances are determined from the time integration of the velocity variances encountered over the history of the puff. The variances are estimated based on the random force theory of turbulent diffusion[5]:

$$\sigma_y^2 = \left[\sigma_{yo}^2 + 2\sigma_{yo} \cdot \delta\sigma \cdot \bar{S} + (\delta\sigma)^2\right], \tag{1}$$

with,

$$\delta\sigma = \sqrt{2} \cdot \sigma_v \cdot t_{Ly}\sqrt{\frac{\Delta t}{t_{Ly}} - 1 + \exp\left(-\frac{\Delta t}{t_{Ly}}\right)}, \tag{2}$$

where σ_{yo} is the spread at the end of the previous time step and the parameter S results from the spatial averaging over the plume width.

RAPTAD was used to make concentration predictions for February 22 for CO, NO_x and SO_2.

PHOTOCHEMICAL MODELING

Description of Photochemical Models

Box modeling of certain episodes was performed to obtain insight into the models performance under MCMA conditions which include higher irradiation and higher photolysis rates than those in the US. Simulations were done with both the Empirical Kinetic Modeling Approach (EKMA) and the box version of the California/Carnegie Institute of Technology (CIT) models. Three chemical mechanisms were used: Carbon Bond IV (CBM-IV)[6] within the EKMA, the Falls, Seinfeld and McRae's mechanism (FSM)[7] and the Lurmann, Carter and Coyner's condensed mechanism[8]. With adjustment to the photolysis constants the three mechanisms showed good performance in the prediction time of the maximum concentration and for the diurnal variation of the pollutants studied. However, the FSM usually gives higher ozone concentrations. The greatest uncertainty for the modeling is the poor information on hydrocarbon speciation which is being addressed in another field program.

The three-dimensional form of The CIT model was then used. The model solves the Atmospheric Diffusion Equation which is a statement of the conservation of species for an ensemble, grid averaged, field. The version used here is a refined, more user-friendly version of the Caltech Model[9,10] and includes gas phase photochemistry and aerosol nitrate formation[12,13]. It uses the LCC mechanism[8]. In a recent study[12] using data from the Southern California Air Quality Study (SCAQS), the model was used to predict ozone, NO2, CO, peroxyacetyl nitrate and individual organic compound dynamics. The application to Mexico City presents a useful opportunity to further evaluate its performance in a very different environment.

Photochemical Model Application

Necessary data for application of an advanced photochemical model to an area like Mexico City include meteorological variables (including a three dimensional wind field, mixing heights, solar insolation and temperatures), geographical characteristics (e.g. elevations and land uses), initial and boundary conditions on concentrations and emissions. This data must be spatially and temporally resolved at the same level as desired for model resolution. Meteorological inputs, except for solar insolation, were developed from HOTMAC. The mixing layers were defined by the heights at which the σ_ws diminished to .1m/s. This description provided a better description of where the random particles moved than did the use of a change in sign of the potential temperature difference. The use of the fluctuations of the vertical velocity is appealing on theoretical grounds, since the vertical velocity fluctuations are the mechanism for vertical mixing. The solar insolation field was derived from measurements within the basin. At this point in the project, the emissions inventory is still being scrutinized, and must be considered preliminary. The inventory used was spatially resolved at the 5 km size, so that scale was chosen for modeling.

COMPARISON OF MODEL RESULTS AND OBSERVATIONS

Wind Predictions

There are several sets of measurements available to test the model results. Figures 2a through d display a comparison of the measured surface winds to the modeled winds for the hours 6am, 10am, 11am, and 12pm. Figure 22b shows that the modeled winds are slow to turnaround in the late morning. In addition the surface winds tend to be too light in the late morning. The evening turnaround was too fast, so that the urban heat island appears to be too strong.

The National Center for Atmospheric Research (NCAR) Beechcraft King Air made a variety of measurements during the February period. Included among the measurements were meteorological parameters: wind speed, wind direction, temperature, and relative humidity, and pollution parameters: CO, NO, NOx, SO2, Ozone and aerosol parameters. In addition the aircraft measured turbulence and radiation parameters including the radiative surface temperature. Other measurements include tethersonde and lidar measurements at the POLY site of figure 1b and the surface measurements. Since the modeled winds are nudged towards the corresponding rawinsonde measurements at the altitudes of one kilometer and two kilometers above the surface, the modeled winds and the measured ones are not completely independent. The winds were generally similar although some differences in speeds and directions were found.

At the polytechnic (POLY) site, the modeled winds were compared to the tethersonde measurements. Overall the directions were fairly good but the modeled winds were too light. The tethersonde winds also showed much more variation in speed and direction than did the rawinsonde winds within the mixed layer. Driving the modeled winds to the rawinsonde winds within the mixed layer may be a mistake because the rawinsonde winds are unlikely to be representative of a several minute average.

The modeled surface temperatures missed the increasing temperatures at the extremes of the NCAR flights (except for the southernmost leg which shows a pronounced drop near an area of wetlands). The rise at the eastern end was probably associated with dry lake areas which are not currently in the model input. The central leg showed higher modeled temperatures over the center of the city, 480 to 490 km easting, than do the observations. This supports the suggestion that the urban canopy description needs to be improved to provide a better timing for the onset of the slope winds.

Mixing Layer Predictions

The lidar indicated that there were significant spatial fluctuations in the apparent height of the mixed layer. In addition there were times when the lidar signal appeared to be dominated by local feature. Overall the lidar measurements suggested that the early morning mixing heights were 200-300 meters rising to 300 to 400 meters at 8:50 and to 400-600 meters at 10:06. The 11:37 value is in the range 800-1200 meters. The modeled values at the same site were 240 meters at 9am, 500 meters at 10am, 830 meters at 11am, and 870 meters at 12 pm. The NCAR aerosol profile for 10:15 suggested a value of about 500 meters.

The tethersonde profiles provided a similar picture of mixing height evolution. Consequently the modeled mixing heights are reasonable representations of the measurements, but further work needs to be done to reduce the uncertainties.

Modeled and Observed Concentrations

Figures 3a through d report early morning to early afternoon hourly SO_2 concentrations in parts per million. The early morning values showed a significant overestimation; small business and commercial sources account for the bulk of the high concentrations. The appropriate temporal behavior for small point sources has received little attention. In addition the early turnaround to downslope winds brings emissions from the evening rush hours back into the urban area. Through mid-morning with the exception of a two points in the north; the predictions are generally similar to the observations. However, later in the day significant overpredictions appear which are probably related to the light winds mentioned previously. The conclusions for CO and NO_x are similar except that there seems to be a tendency for the model to underestimate morning NOx concentrations.

Figures 4a through c compare the NCAR observations of SO_2, CO, and NO_x with modeled values for the ascent of Feb. 22. This flight was about 10am. The model calculations are actually for the Polytechnic site. The modeled profiles are similar to the measured ones and it is interesting to note the differences in the shape of the profiles between the various pollutants.

Comparison between measured and modeled ozone

Results of the preliminary application of the CIT model to the 22 February 1990 measurement period are shown in figures 5a through f. The model is found to follow the dynamics of the ozone well at those sites. Predicted afternoon ozone levels at a number of sites did not drop as rapidly as the measurements show. This is likely due to either lower inventoried NO emissions than are actually present, or that the vertical mixing is more rapid than actual. The NO emissions inventory showed significant spatial variations, and this can lead to steep concentration gradients. It was found that both the model predictions and measurements show very steep horizontal ozone concentration gradients. The peak predicted ozone (0.29 ppm) was 25 km from the peak measured ozone concentration (0.33 ppm). Given the preliminary nature of the inventory, and that there are some uncertainties in prediction of the meteorological variables, this level of agreement is good. Further evaluation will be conducted when an updated inventory is available, but the preliminary results are quite encouraging that the transport variables (e.g. winds and mixing depths) are in good shape.

SUMMARY

A joint study of Mexico City's air quality problems between Los Alamos National Laboratory and the Instituto Mexicano Del Petroleo is underway. The model uses a three-dimensional prognostic meteorological code to provide wind and turbulence fields to a Monte Carlo kernel, random particle transport code. A model of this sophistication was chosen because of the important terrain influences in the region and the limited meteorological data. The meteorological model output is used to drive the CIT photochemical model. The modeling system was used to make predictions for one day which displayed a typical pattern of poor air quality. A variety of measurements by aircraft, surface networks, tethersonde, lidar and rawinsonde were conducted to test the model and provide information about model deficiencies. Predictions were made and compared to experiments for winds and concentrations of CO, NO_x, ozone and SO_2.

The modeling system shows promise for addressing the air quality questions, but there are also deficiencies in its application. One of the deficiencies was an urban heat island which was too strong, so that the morning slope winds were too late and the afternoon ones too early. Another deficiency was high predictions of early morning concentrations. Additional studies now underway will provide an opportunity to improve the model and the input data for this application.

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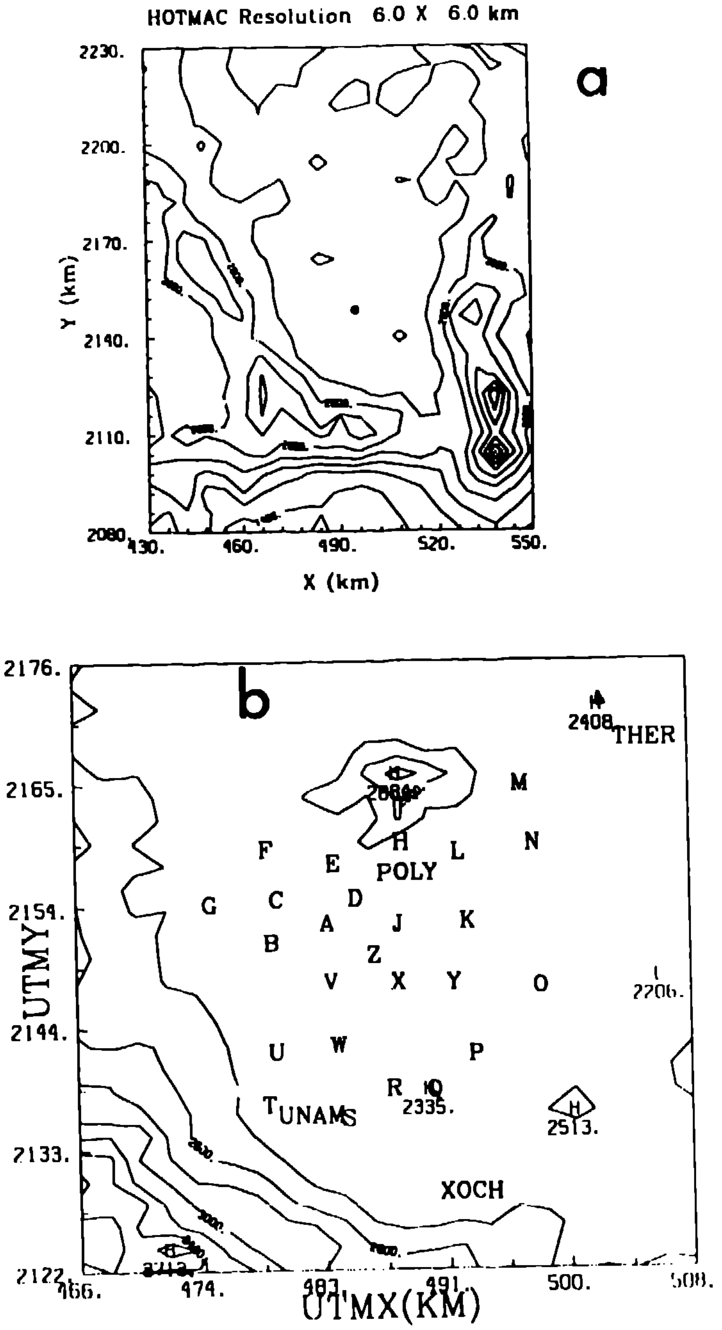

Figure 1: (a) Coarse grid depiction of the model domain; the dot is the airport on the east-side of the city. (b) Fine grid depiction of the model domain. The letters denote Sedue monitoring sites, while POLY, THER,UNAM, and XOCH denote lidar sites.

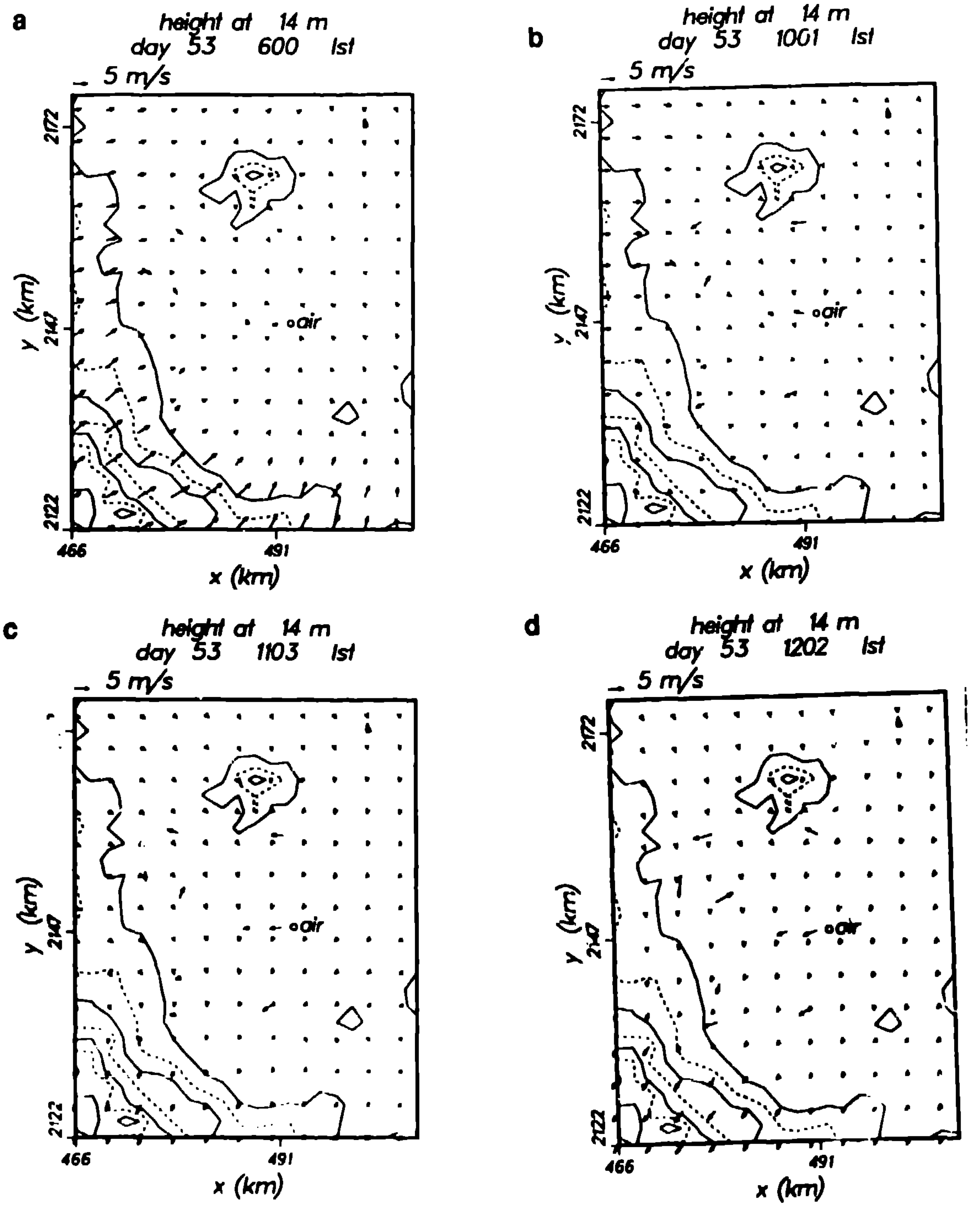

Figure 2: Comparison of modeled winds with surface measurements on Feb. 22, 1991 at (a) 6am, (b) 10am, (c) 11am, (d) 12pm. Measured values are plotted at actual locations while the calculated values are at regularly spaced grid points. Air denotes the airport.

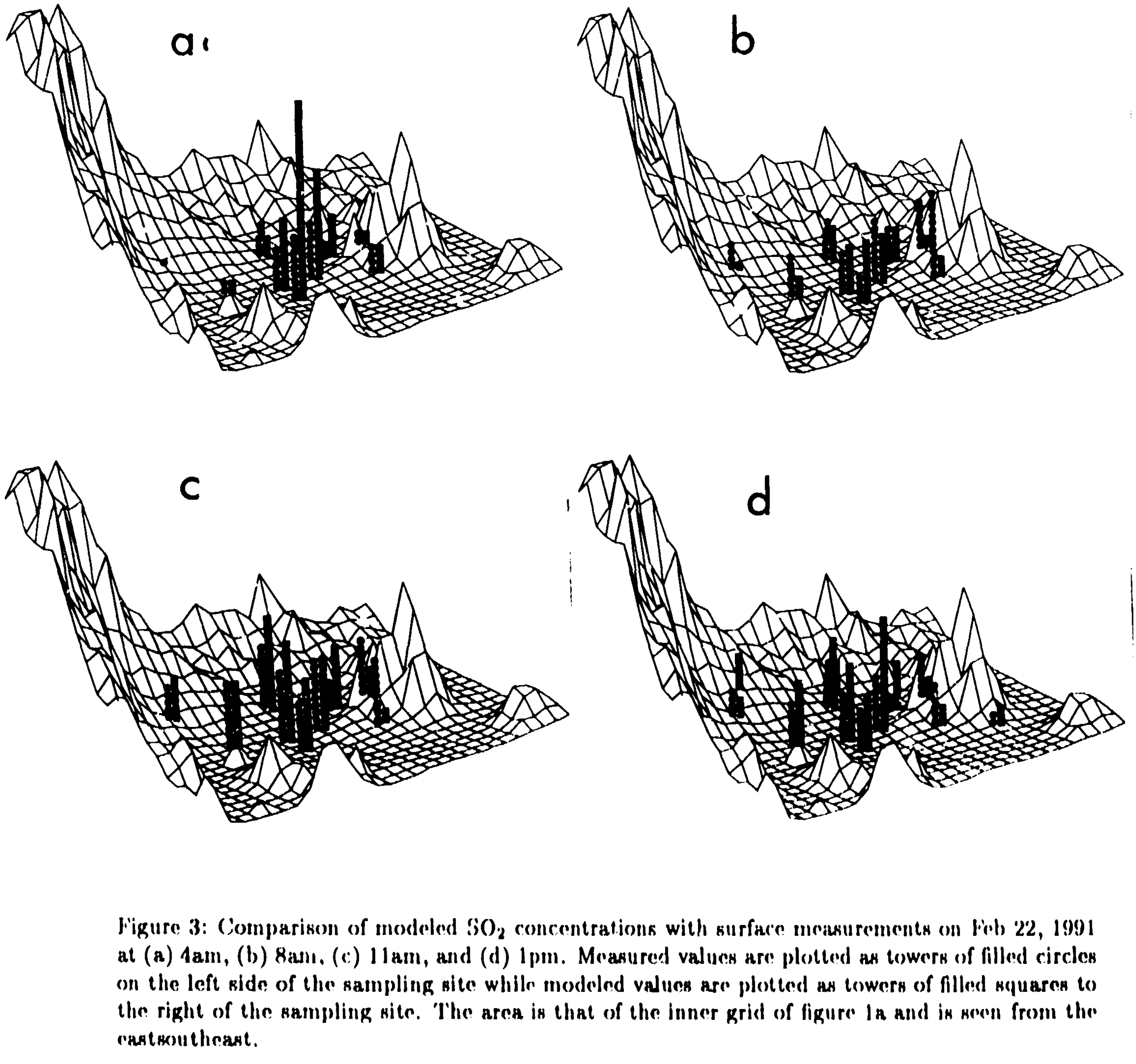

Figure 3: Comparison of modeled SO_2 concentrations with surface measurements on Feb 22, 1991 at (a) 4am, (b) 8am, (c) 11am, and (d) 1pm. Measured values are plotted as towers of filled circles on the left side of the sampling site while modeled values are plotted as towers of filled squares to the right of the sampling site. The area is that of the inner grid of figure 1a and is seen from the eastsoutheast.

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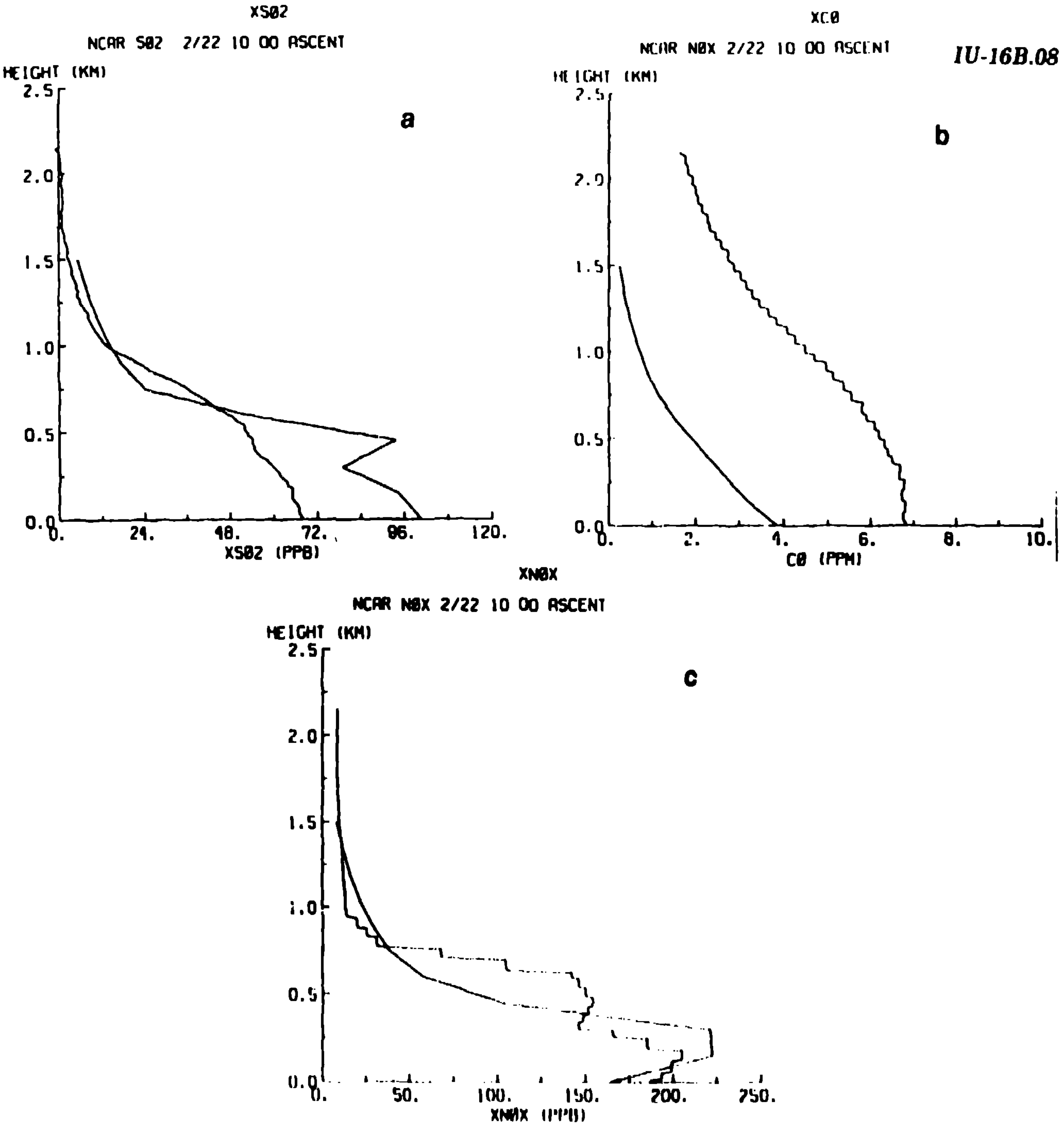

Figure 4: Comparison of modeled and NCAR aircraft concentration profiles at 10am on Feb. 22, 1991 for (a) SO_2 , (b) NO_x, and (c) CO. NCAR measurements are the more jagged lines.