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METEOROLOGICAL AND SULPHUR DIOXIDE DISPERSION MODELLING FOR AN INDUSTRIAL COMPLEX NEAR MEXICO CITY METROPOLITAN AREA

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Major sulphur dioxide emissions in Mexico are due largely to fuel of oil refining and coal combustion. In Tula-Vito-Apasco industrial corridor (TVA) are located two important sources of SO_2: the “Miguel Hidalgo” refinery and the “Francisco Perez Rios” power plant. Due to from March 25 to April 22 of 2006 a major field campaign took place as part of a collaborative research program called MILAGRO. Data collected around the Industrial Complex were used to: a) evaluate the air quality to local and regional scale; b) study the structure of the atmospheric boundary layer (BL); and c) validate meteorological and dispersion models. In this study we presented the behaviour of daytime BL, and the results of meteorological and dispersion modelling for selected episodes of high sulfur dioxide (SO_2). The Regional Atmospheric Modeling System (RAMS) and the Hybrid and Particle Concentration Transport Model (HYPACT) were used to evaluate the impact of SO_2 emissions to regional scale. For modelling, we selected the days where higher mean daily levels of SO_2 surface concentrations were observed, these corresponded to March 31 and April 6. The results indicate that: (1) The daytime BL in TVA, exhibited a normal behavior, a stable layer or thermal inversion close to surface was observed at 0800 LST (up to 80% of the cases), then the mixing height (MH) growths, with a growth rate of 313 m h^{-1} (between 0800 to1200 LST). The most rapid MH growth happened between 1200 to 1500 LST; (2). The maximum MH was observed at 1500 LST (90% of the cases); the mean maximum MH was close to 2794 m AGL; (3) Potential temperature and humidity profiles showed a normal behavior; (4) High persistence in wind direction (> 0.6) close to surface up to 500 m AGL, was observed at 1500, and 1800 LST, at the same time, a low level jet, penetrating from the NE, with wind speed between 6 to 8 m s^{-1} was observed. Meteorological modelling was used to determine the circulation patterns in the region, and as input to dispersion modelling. Validation of the meteorological model was focused in the variables used as input in the dispersion model, consequently simulated and observed values of profiles of wind speed and direction, potential temperature, and specific humidity and were compared. RAMS mixing heights were overestimated at late morning (0800 LST), but during the afternoon were found to be in good agreement with observations. Simulated potential temperature and specific humidity profiles showed good agreement with the corresponding observed profiles. Simulated wind speed profiles and surface winds presented similar behavior that observations, but surface wind speed was overestimated at late morning and underestimated at the early evening. HYPACT simulations indicate that air quality standard for SO_2 (=0.13 ppm or 341μgm^{-3} in 24 hours) was exceed close to source emissions. Models simulations indicate that TVA emissions can reach the Mexico City. HYPACT performed well the general behaviour of surface concentrations of SO_2 but fails to simulate the observed peaks of the pollutant.

Keywords: Air pollution, Mexico city, Lagrangian model, Industrial emissions

1. Introduction

Air pollution problems in Mexico show a distinct relation between pollution, complex topography, and the size and dynamics of human settlements. Although 40% of the total atmospheric emissions in the country are generated in the metropolitan areas of the cities of Mexico, Guadalajara y Monterrey, some smaller cities has serious air pollution problems too, due to the high concentration of industries as occur in the region known as the Tula-Vito-Apasco (TVA) industrial corridor. Oil refining, power generation, petrochemical, cement and mining industry are the principal responsible of SO_2 emissions in the TVA industrial corridor. Two important sources of SO_2: located in TVA are the “Miguel Hidalgo” refinery and the “Francisco Perez Rios” power plant, which contributing almost 90% from the total emissions of SO_2 inside the Hidalgo State. The Environmental Authorities has classified the TVA industrial corridor as a critical zone due to its proximity to Mexico City, and the elevated concentrations of atmospheric pollutants observed.

The Tula-Vito-Apasco industrial corridor is located in the Mexican state of Hidalgo, in an elevated basin (on average 2100 m above mean sea level) in Central Mexico (20.05°N and 99.27°W). It is surrounded by low hills but with an

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opening to the southeast. The hills located to the east, west, and north rise 200 or 300 m above the basin, but with lower terrain on either side. The TVA is located 70 km to the north-northwest of the Mexico City.

In order to evaluate air quality in the TVA the Instituto Mexicano del Petroleo (Mexican Petroleum Institute, IMP) since last 1990´s has conducted a series of field campaigns in the region focusing on surface air quality and emissions measurements. Data collecting has been used in Gaussian modelling or statistical analysis to study the tendency or air quality.

During March 2006 a big research program was conducted Megacity Initiative: Local and Global Research Observations study (MILAGRO). The goal of MILAGRO [1] was to study the atmospheric processes leading the formation of secondary aerosols and their transport on local, regional, and global scale. MILAGRO joined several researchers from different parts of the world. As part of this project a field campaign was conducted by the IMP in order to obtain data to determine the BL evolution in the TVA, particles chemical composition, and as input to modelling to evaluate the impact of TVA´s emissions on the Mexico City Metropolitan Area (MCMA) air quality.

The behaviour of the daytime mixing height and modelling results of two high sulphur dioxide episodes are presented in this paper.

2. Data and Methodology

2.1 Data and synoptic overview

The synoptic conditions during the field campaign were variable. At the beginning of the field campaign the pass of a well-developed trough was observed producing overcast conditions during March 18-19. From the period March 24-27, the intrusion of a “Norte” (Northern or cold surge) generated overcast conditions and light to moderate rain after noon. During April the most of the days were clean or near-cloudless skies, without rain observed, due to the presence of high pressure systems.

Wind direction at 500 hPa at 12 GTM was from 5 directions: 45.2% southwesterly (SW), 35% westerly (W), 13 % northeasterly (NE), and 3.2% correspond to south (S) and northwesterly (NW) winds, respectively.

Most of the days, the maximum temperature was over 22°C, only during the period of March 24-26 the maximum temperature was close to 18 °C. Wind speeds at surface varying form light to moderate were observed.

The surface and upper-air meteorological data used in this study were obtained during the special field campaign conducted by the IMP that took place in Tula from March 18 to April 22, 2006. This field campaign was part of the MILAGRO study that took part during March 2006.

During the campaign in Tula, four rawinsondes per day were launched at 0800, 1200, 1500, and 1800 LST. Also two surface stations at Jasso, and Tepeji were deployed to measure meteorological, and air quality variables. Figure 1 shows topography, and the location of the stations used in this study.

2.2. Methodology

Rawindsondes measured temperature, wet bulb temperature, pressure, and wind. From these, the potential temperature, and mixing ratio were calculated. Data were interpolated each 5 hPa, before to obtain the average temperature, humidity, and wind profiles. All available data were used.

The mean wind profiles were calculated considering its vectorial character. In order to determine the representativeness of the wind profiles the wind persistence was calculated. Wind persistence is defined as the ration of the mean vectorial wind speed and the mean scalar wind speed. High values of the ratio indicate that wind has little changes in direction, but low values indicate large variations in wind direction.

To calculate the mixing height, the profiles of potential temperature and mixing ratio were plotted, and the height of the mixing layer was identified with the base of an elevated capping inversion or stable layer, and when a significant reduction in air moisture occurred (Seibert et al., 2000). The growth rate of mixing height was calculated as the ration between the change of the mixing height and the time-height variation (i.e., MH growth rate $=\Delta MH/\Delta t$). When we have more than one site to calculate the mixing height growth rate, we obtained a mean value of the MH growth rate.

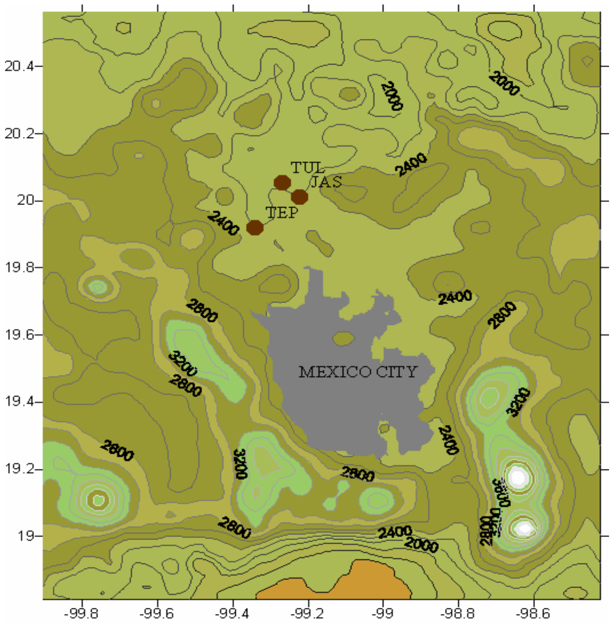


Figure 1. Topography of Tula-Vito-Apasco and Mexico City region. The topography contour interval is 200 m. Location of the rawinsonde station (Tula, TUL), and locations of surface stations (Tepeji, TEP, and Jasso, JAS).

All the days of the field campaign were examined in order to determine the days when the peak of sulfur dioxide (SO_2) occurred, and wind circulation indicated a possible impact of TVA emissions in the air quality of the MCMA. The selected days are March 31 and April 6.

A mesoscale meteorological and dispersion simulation is performed for each day selected. Each simulation starts at 0000 LST and last for 72 hours, with the second afternoon being the period of interest. This is done in order to examine the relative contribution of the previous day's emissions to near-surface concentrations.

The emissions inventory of the Hidalgo Sate is used to determine the SO_2 emissions corresponding to energy sector, oil and petrochemical industry, and mining industry. Emissions used in modelling were grouped according to the stack height and flux emission temperature resulting in 18 points of emission, which two of them represent the "Francisco Pérez" power station´s emissions, 4 represent "Miguel Hidalgo" refinery's emissions; and the rest are emissions from mining and cement industry.

3. Model Description

The RAMS-HYPACT modelling system was used to investigate the effect of local and regional flows in the spatial distribution of sulphur dioxide (SO_2) and the impact in the air quality of Mexico City.

3.1. Meteorological model

The Regional Atmospheric Modelling System (RAMS) is a primitive equation, nonhydrostatic model based on a terrain-following coordinate system. Sub-grid turbulent diffusion is parameterized using a level 2.5 scheme: turbulent and sensible and latent heat fluxes and momentum in the surface layer are evaluated based on Louis's formulation. The Chen and Cotton shortwave and longwave scheme is used. Despite of RAMS contains both cloud microphysics package and a cumulus parameterization scheme neither of them were activated in this study [2, 3].

The modelling domain consists of three nested grids with horizontal grid spacing of 32, 8, and 2 km. The outer grid encompasses most of Mexico and parts of the Gulf of Mexico and Pacific Ocean. The inner grid encompasses the Tepeji-Tula-Apasco region and the Mexico City basin. By employing a nested grid configuration, the effects of the synoptic-scale flows on local and regional flows can be represented. A stretched grid is used in the vertical coordinate with a stretching ration of 1.2, starting with a grid spacing of 50 adjacent to surface. As a result 26 points grid points are located in the first 4 km above ground level, when maximum resolution to resolve boundary layer processes is required. The top of the model is at the elevation of 23 km. The model domain and the topography in the inner grid are showed in Figure 2.

Four data assimilation each 3 hours of surface data, and 4 times per day upper air meteorology (0000, 1200, 1500, 1800 LST, rawinsondes launched in Tula) as well as the standard upper-air soundings at Mexico City, Guadalajara, Veracruz, Acapulco and Monterrey were incorporated to the model. Also, global data from the US- National Center of Environmental Prediction (NCEP) with 2.5 degree spacing were used in the model simulations. The resulting meteorological fields were mesoscale analysis, which combine the predicted and observed variables when and where observations were available.

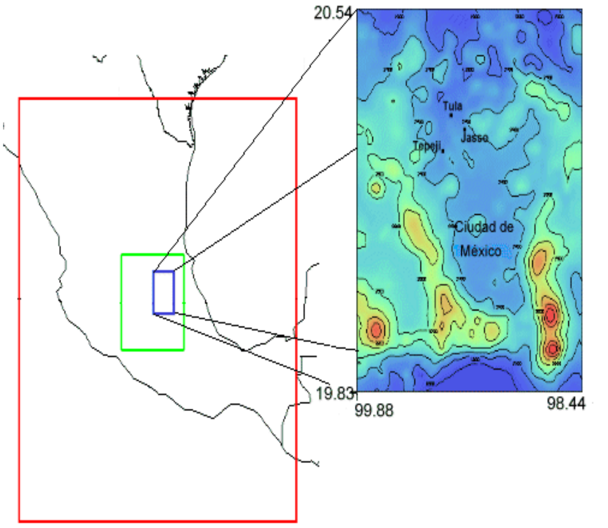


Figure 2. RAMS model domain and topography (black lines) in the inner grid.

3.2. Dispersion model

The HYPACT (Hybrid Particle And Concentration Transport Model, [4, 5]) is a code developed to simulate the motion of atmospheric tracers under the influence of winds and turbulence. HYPACT combines in one code the Lagrangian and Eulerian dispersion estimating methodologies. Its Lagrangian component enables representation of sources of any size, and the maintenance of concentrated, narrow plumes until atmospheric dispersion dictates that it should broaden. At this point, the Lagrangian particle plume can be converted into a concentration field and then advected using an Eulerian formulation. The Lagrangian particles are moved through space and time based on the interpolated wind velocities plus a superimposed random motion scaled on the local turbulent intensity. Additionally, a spectrum of gravitational settling velocities related to particle size can be specified. Wind components, potential temperature, and turbulent kinetic energy are the gridded meteorological variables necessary to drive HYPACT. For this project, gridded time series of these variables are provided by the RAMS model to HYPACT.

The HYPACT model has the same domain configuration that the RAMS inner nested grid. For this study, the Lagrangian mode of HYPACT was configured to run only for the inner grid of the RAMS model. Particles representing the emissions of SO_2 from the different sources were released at a rate of 20 per time step of 100 s.

For the present study, HYPACT was initialized at 0000 LST and the duration of the simulation was 72 hours, the period of interest is the second afternoon day. Emissions are continuous source.

4. Results

4.1. Observed characteristics of the boundary layer evolution

4.1.1. Mean temperature and humidity profiles

Figure 3 shows the mean potential and specific humidity; both of them exhibit a normal behaviour. During 80% of the days in the campaign, at 0800 LST a stable layer (sometimes with a thermal inversion) close to surface was observed. At 1200 LST, the stable layer was eroded and a shallow super adiabatic layer with a mixing layer close to 2000 m AGL is observed.

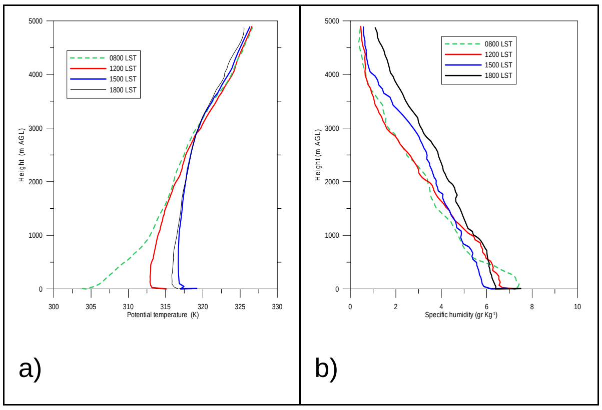


Figure 3. Mean potential temperature (a) and specific humidity profiles (b), at the Tula site.

The potential temperature profiles at 1500 and 1800 LST were similar above 500 m. However, close to surface the potential temperature profile at 1800 LST was colder than the potential temperature profile at 1500 LST indicating the formation of a stable layer close to surface (see Figure 3a).

Meanwhile the specific humidity profiles indicate a normal behaviour, showing a reduction of humidity with the height. The humidity difference between each humidity profile was less than 4.0 gr Kg^{-1}. See Figure 3 (b).

The height of the mixing layer (ML) varied significantly from one day to another. On some days the depth of the ML was upto 4200 m AGL, but in other days it was lower than 2500 m AGL. Special cases were the days March 24 and 25, when maximum daily MH was lower than 500 m AGL.

Despite of the mixing height (MH) variation from one day to another, the growth of the ML depth during a diurnal cycle exhibited typical characteristics. At 0800 LST, a stable layer (in some cases with thermal inversion) was observed in 80% of the cases. When the stable layer or thermal inversion does not exist, MH varied from 38 to 380 m AGL. As the day progress, MH growths about 313 m h^{-1}, to reach a mean value close to 1375 m h^{-1} at 1200 LST. Between 1200 and 1500 LST was observed a rapid growth of the MH, with a growth rate of about 470 m h^{-1}. ML depth between 1500 and 1800 LST, presented a decrease rate about 72 m h^{-1}.

Diurnal maximum MH was observed, in the majority of the cases, at 1500 LST. The daytime boundary layer behaviour in Tula can be seen clearly in Figure 4.

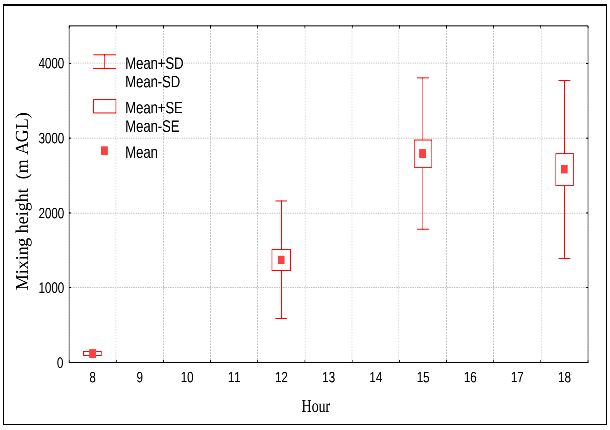
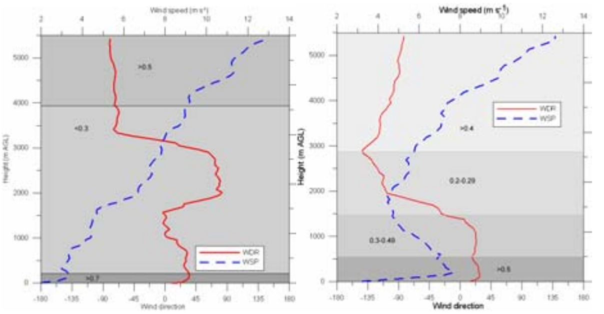


Figure 4. Mixing height behaviour at the Tula site, during March-April, 2006.

4.1.2. Mean wind profiles

Figure 5 shows the mean vector winds, calculated from rawinsondes launched at 1200 and 1500 LST for the total period of the field campaign. In the figure, the persistence of the day to day winds, the ratio of the vector mean wind speed to scalar mean wind speed is indicated in gray shades. The Figure 2a shows that the mean winds (1200 LST) below 300 m AGL are very regular and light blowing from the northeast; up this height, winds were variable. The wind speed increases constantly with height, but wind direction keeps constant to 1800 m AGL, then it veers to the east and keeps constant to about 3000 m AGL. The wind persistence at 0800 LST (not show here) indicate a regular behavior close to 100 m AGL with wind blowing form the south-southwest.



a) 12 LST b) 15 LST

Figure 5. Mean Wind profiles at the Tula site, March-April, 2006.

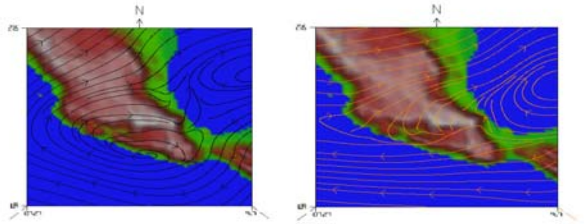
Higher wind persistence close to surface was observed at 1500 LST varying from 0.66 to 0.86. The mean wind direction was from the northeast, and it keeps constant to a height close to 1500 m, and then it veers to flowing form the west-southwest. At the same period time, the wind speed shows a logarithmic profile in MH, with a maximum value close to 6 ms^{-1} at 500 m of height.

The mean wind profile at 1800 LST (not show here) is similar to the wind profile at 1500 LST, but maximum wind speed (7.0 m s^{-1}) is observed at 250 m of height.

4.2. Modelling results

4.2.1. Meteorological fields

Figure 6 shows the synoptic weather conditions at 700 hPa on March 31 and April 6. A high pressure system centered over south of Mexico may be responsible of the moderate northwesterly winds observed in the region of interest. The westerly winds at 700 hPa are result of another high pressure system located over the central Gulf of Mexico on April 6. Along the day wind speed is higher on March 31 than April 6. Observed wind speed on March 31 varying form light (<5 ms^{-1}) to moderate (5 to 8 ms^{-1}); meanwhile on April 6 wind speed was light. Observed maximum temperature was 5°C higher on April 6 than March 31.



March 31 April 6

Figure 6. The 700 hPa streamlines at 1200 UTC (0600 LST) from model inizalitation.

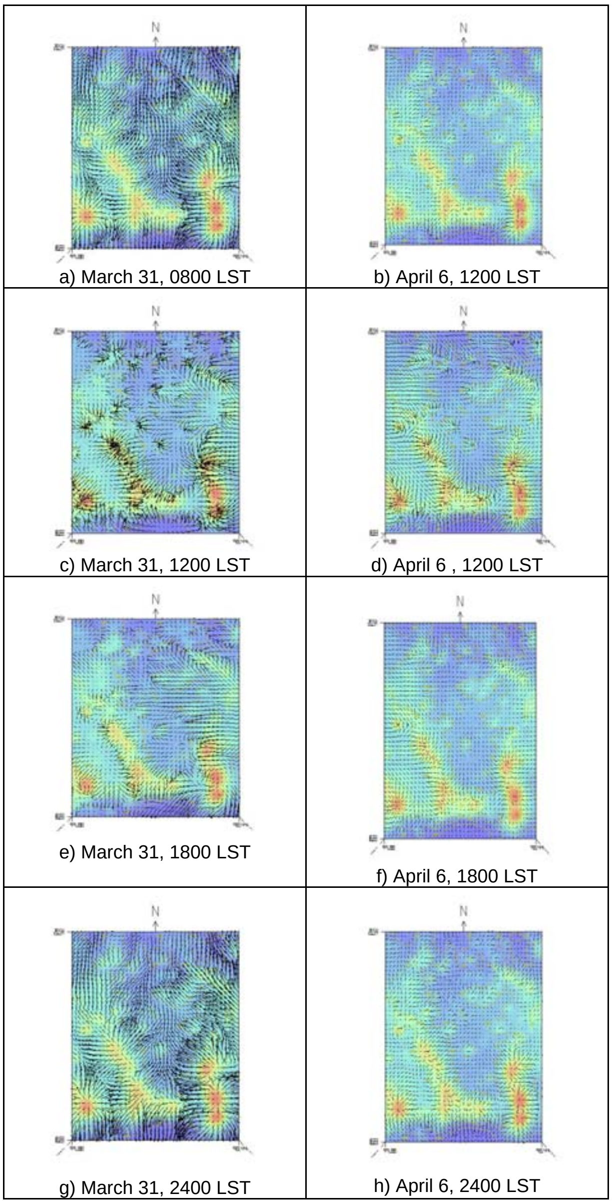


Figure 7. Near-surface wind flows.

The simulate near-surface wind fields at four times on March 31 and April 6 are shown in the Figure 7. As is expected, thermally driven flows developed in the region in response to the daytime heating. Despite of similar synoptic conditions on March 31 and April 6 wind patterns near surface are different at noon and evening, but very similar in the early morning and night. In the early morning and midnight the down-slope wind flows to the northern end of the basin. At 1200 LST on March 31 can be observed up-slope winds well-developed in the MCMA but not in the TVA region where the winds are light and not show a defined pattern. On 6 April, at the same time period, in the TVA region westerly winds are observed, meanwhile in the MCMA similar wind patters than previous described are observed. On March 31 the near-surface winds field at 1800 LST are still up-slope along of the west side of the basin. Something different happens on April 6, where down-slope winds converge to the northern end of the MCMA.

Its seem that near-surface wind flows in the TVA region, when synoptic forcing is light, is directly influence by local topography generating local wind circulations as its seem on March 31, but if convective boundary layer is warmer in the MCMA than in the TVA region a temperature and pressure gradient is generate after noon causing that the winds flows in the TVA region are alienated to the winds flows in the MCMA, as occurred on April 6.

4.2.2. Dispersion

The HYPACT model run in a Lagrangian configuration in order to examine the transport characteristics associated with meteorological processes. Dispersion simulation started 24 hours previous the period of interest. Figure 8 shows the SO_2 isosurface during the episode days. An isosurface shows the 3D volume bounded by a particular isovalue; the volume inside contains values greater than the isovalue. An isosuface allows studying plume behaviour in 3D.

On March 31, in the early morning the plume dispersion flows to the northern end of the model domain due to the influence of down-slope winds. At 1200 LST, when the up-slope are well defined the plume dispersion veer and a recirculation of SO_2 in the TVA was observed without impact the MCMA. At midnight, most of the emissions were in the residual boundary layer, so the plume dispersion again is to the northern end of model domain. See Figure 8.

In the early morning, on April 6 the plume dispersion has different behaviour as was described previously. Previous day recirculation of SO_2 (observed in Figure 8) contributed to the accumulation of SO_2. In the early morning two plumes were clearly observed due to different wind direction in the residual boundary layer. When the wind direction in boundary layer was similar the plume dispersion was narrow and flowed to NE. After noon, the wind blows from the NE veering the plume dispersion and reaching the MCMA. At midnight the plume veers again to the north-eastern end of model domain. High of the plume dispersion was low to 1000 m (not shown here).

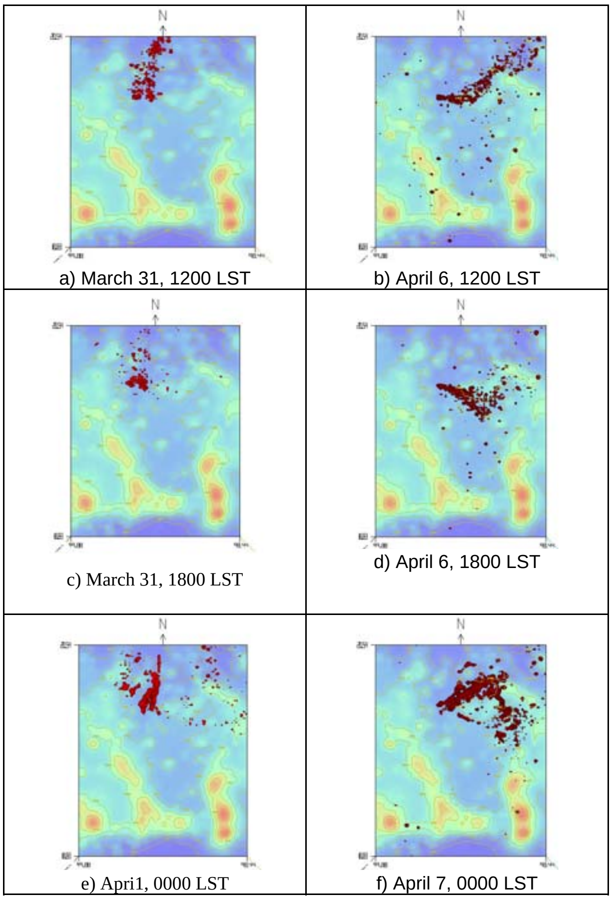


Figure 8. Sulphur dioxide isosurfaces (0.219 ppm) on March 31 and April 6, 2006.

Despite of high level of SO_2 observed in the plume dispersion, the 24-hour mean SO_2 near-surface concentrations were up the standard regulation (= 0.13 ppm or 341 μgm^{-3}) only close to the source emissions as is shown in the Figure 9.

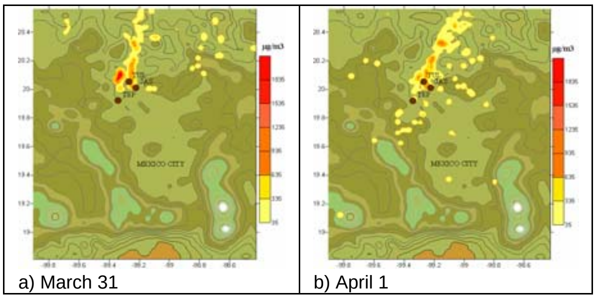


Figure 9. The 24-hour mean SO_2 near-surface concentrations, 1500 LST.

The 24-hour mean SO_2 near-surface concentrations correspond to 1500 LST, when the maximum concentration where observed.

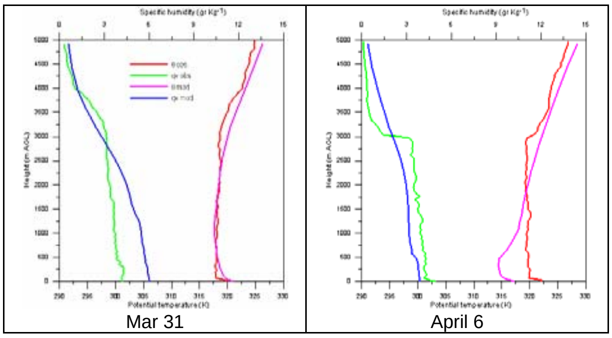


Figure 10. Observed and simulate potential temperature and specific humidity profiles, at 1500 LST, at the Tula site.

4.2.3. Model validation

Simulated and observed values of profiles of wind speed and direction, potential temperature, specific humidity and surface meteorological variables are compared for 1 site with upper meteorology. The RAMS mixing heights were overestimated at late morning, but during the afternoon were found to be in good agreement with observations (not shown here). Simulated potential temperature and specific humidity profiles showed good agreement with the corresponding observed profiles as shows Figure 11. Simulated wind speed profiles reproduced the intrusion of the low level at the afternoon (see Figure 11). The wind speed was overestimated at late morning and underestimated at the early evening. Model better results were obtained on March 31 than April 6.

Figure 12 shows the observed and simulated near-surface SO_2 concentrations at the Tepeji site. The hourly SO_2 behaviour is well represented but not the observed peaks of SO_2. On 31 March the near-surface SO_2 concentrations are under-estimating. On the contrary, on April 6 the near-surface SO_2 concentrations are overestimate.

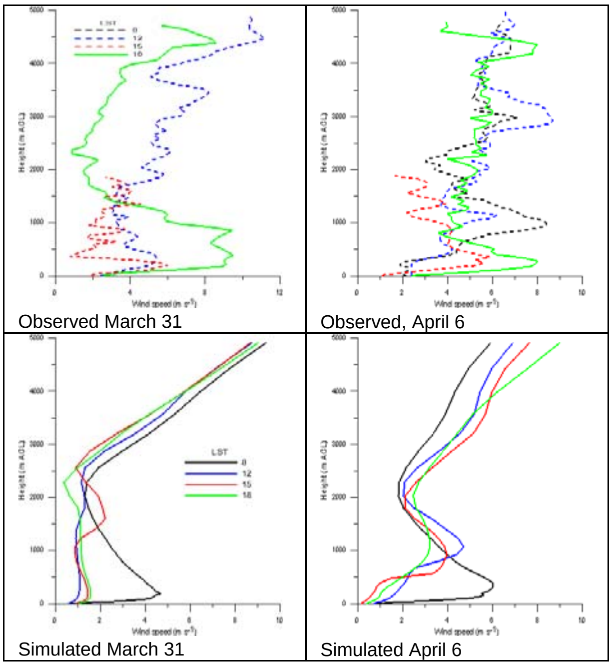


Figure11. Observed and simulate wind speed profiles, at the Tula site.

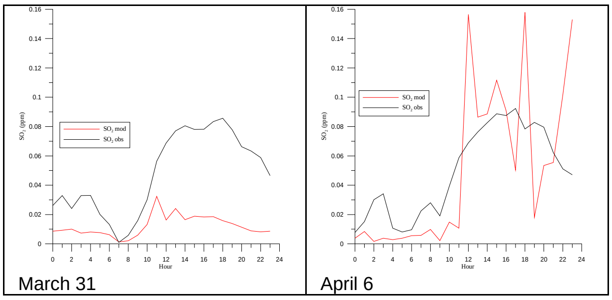


Figure12. Observed and simulated near-surface SO_2 concentrations at the Tepeji site.

5. Conclusions

This study was focused to determine the daytime boundary layer in the TVA industrial corridor and modelling results of two high sulphur dioxide episodes are presented in this paper.

We found that the day time BL in TVA, exhibited a normal behavior, a stable layer or thermal inversion close to surface was observed at 0800 LST (upto 80% of the cases).The most rapid MH growth happened between 1200 to 1500 LST; (2). The maximum MH was observed at 1500 LST (90% of the cases); the mean maximum MH was close to 2794 m AGL.

High persistence in wind direction (> 0.6) close to surface upto 500 m AGL, was observed at 1500, and 1800 LST, at the same time, a low level jet, penetrating from the NE, with wind speed between 6 to 8 m s^{-1} was observed. This low level jet has not been previously observed.

Simulated potential temperature and specific humidity profiles showed good agreement with the corresponding observed profiles. Simulated wind speed profiles reproduced the intrusion of the low level at the afternoon (see Figure 12). The wind speed was overestimated at late morning and underestimated at the early evening.

Models simulations indicate that TVA emissions can reach the Mexico City but in low concentrations.

The 24-hour mean SO_2 near-surface concentrations were up the standard regulation (= 0.13 ppm or 341 µgm^{-3}) only close to the source emissions.

The general behaviour of surface concentrations of SO_2 was well simulated but model fails to simulate the observed peaks of the pollutant.

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