P1.9 AN EXAMINATION OF AIR QUALITY MEASUREMENTS AND SIMULATIONS OVER MEXICO CITY, MEXICO AND HOUSTON, TEXAS

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1. ABSTRACT

Atmospheric composition, aerosol optical depth, and air particle trajectories were analyzed to assess the agreement of instruments and models, and create a temporal analysis of air quality in Mexico City, Mexico and Houston, Texas. The variation and concentration of ozone and nitrogen dioxide levels was investigated using model, satellite, and in situ data sources. Additionally, an algorithm was created to find coincident data points between model, satellite, and airborne data sources to analyze aerosol optical depth. Furthermore, a comparison of a trajectory model with an in situ based trajectory model described air movement in the study region. For March 2006, a STEM and ozonesonde time series for Houston showed a correlation of 0.62. When comparing ozonesondes with TES on 7 and 23 March 2006, percent error values were 1.3% and 24% respectively. An analysis of aerosol optical depth comparing HSRL and MODIS on 7, 12, and 13 March 2006 indicated significant correlation with R-values of 0.87, 0.74, and 0.53 respectively. A comparison of WRF-CHEM to HSRL on 7 and 12 March showed correlation values of 0.57 and 0.84 respectively. A comparison of WRF-CHEM to MODIS on the 7th, 12th, and 13th showed correlation values of 0.34, 0.23, and 0.08 respectively. It is essential to validate models and instruments to provide the highest level of accuracy for the scientific study of aerosols and other atmospheric chemicals.

2. INTRODUCTION

With growing concerns over changing atmospheric and climatic conditions, researchers around the world are exploring new methods of assessing aerosol distribution. High concentrations of atmospheric pollutants are detrimental to public well being because of increased levels of tropospheric ozone and reduced visibility. Visibility reduction in rural and urban areas is primarily the result of high turbidity due to aerosols (Marquez et al., 2005). According to the American Lung Association, aerosol pollutants may be linked to cardiovascular, respiratory, and neurological damage to the human body. By infiltrating the lungs and blood stream, elevated levels of aerosols can hinder oxygen in reaching vital organs. If the brain is affected, learning impairment and slow judgment may cause a loss of productivity (American Lung Association, 2002). High concentrations of ozone and aerosols damage the human respiratory system (Cheng et al., 2006; Bravo et al., 2002) and can be carcinogenic when inhaled (Baumgardner et al., 2000).

According to Atmospheric Environment, mega-cities worldwide account for substantial aerosol loading due to the large number of inhabitants and localized emissions. Mexico City is one of the largest mega-cities in the world and sustains elevated anthropogenic aerosol concentrations (Raga et al., 2001). The topography surrounding Mexico City traps aerosols because the location is bordered by two mountain ranges to the southeast and southwest. The mountain ranges act as barriers restricting ventilation of emissions (Villasenor et al., 2003; Bravo et al., 2002).

Population centers downwind of Mexico City are influenced by polluted outflow (He et al., 2006). Marquez (2005) reports anthropogenic particles and gases at Pico de Orizaba National Park, approximately two hundred miles southeast from where they originated in Mexico City. Oxidation intermediates have also been reported in the Mexico City outflow (Madronich, 2005). Pollution outflow may cause a large-scale hazard to ecosystems and communities.

The INTEX-B (INtercontinental chemical Transport EXperiment B) campaign was one of four experiments in the MILAGRO (Megacity Initiative: Local and Global Research Observations) campaign. Two instruments employed during the INTEX-B campaign were the NASA Langley airborne High Spectral Resolution Lidar (HSRL) and the MODerate Resolution Imaging Spectroradiometer (MODIS) instrument. The HSRL accurately measures profiles of aerosol extinction with high vertical resolution (Hostetler et al., 2006). The MODIS instrument measures atmospheric aerosols and can be combined with ground-based and airborne observations for a more comprehensive analysis (Hutchison et al., 2005). This paper describes how the MODIS and HSRL measurements were compared and utilized to examine forecasted simulations of aerosol optical depth (AOD) provided by the Weather Research and Forecasting model (WRF) coupled with the Regional Atmospheric Chemistry model (RACM) chemical mechanism (referred to hereafter as WRF-Chem), and the Sulfur Transport Eulerian Model (STEM).

We also compare STEM predicted levels of tropospheric ozone and tropospheric ozone precursor, nitrogen dioxide, between Mexico City and another city recognized by NASA as having, “a serious air quality problem,” Houston, Texas (Wilson, 2007). A further investigation of the air pollution issue in issue consists of a comparison between measured values from ozonesondes and the Tropospheric Emission Spectrometer (TES), an instrument aboard the NASA Aura satellite.

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Finally, we performed a preliminary investigation into air trajectory modeling. We compared NOAA's HYbrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) model to Florida State University's in situ based trajectory model. Being able to demonstrate the accuracy of HYSPLIT, coupled with its ease of use, will provide support for a more in-depth study of air movement in our study region.

3. METHODOLOGY

3.1 *Houston Ozonesonde Data compared with STEM and TES*

Ozonesonde data over Houston, obtained from Rice and Valparaiso Universities, were compared with STEM during March 2006. Ground-level STEM simulations were plotted against surface ozone measurements for all available days in March. STEM ozone concentrations averaged between ground level and 1 km were temporally averaged between 18 and 21 UTC model runs given that most ozonesonde launches occurred approximately between 18 and 19 UTC. The generated STEM ozone concentration set was plotted as a function of 1-km column-averaged ozonesonde measurements as to be comparable the 1-km averaged STEM concentrations. Ozonesonde data over Houston were compared with column averaged ozone concentrations obtained from TES. The days of 7 and 23 March 2006 were selected as having the best satellite overpasses for a comparison to ozonesonde column average concentrations. For the selected days, the ozonesonde measurements were averaged to the maximum launch height attained by the balloon, 21.3 and 29.3 km for 7 and 23 March, respectively. The TES data were averaged to the same altitude.

3.2 *STEM tropospheric ozone for Mexico City and Houston, TX*

The air quality analysis for Mexico City and Houston focused on ozone (O_3) and nitrogen dioxide (NO_2). The latter compound is both a precursor and a byproduct of tropospheric ozone formation. For Mexico City, STEM data for each compound were analyzed daily at 06, 12, 18, and 21 UTC from 1 to 31 March 2006. A similar analysis was conducted for Houston, but the times of 00, 06, 12, and 18 UTC were used.

3.3 HSRL, MODIS, and WRF-Chem data

Further data were acquired from WRF-Chem. The MILAGRO campaign presented a unique opportunity for aerosol assessment using several models and instruments. Aerosol optical depth measurements from the MODIS instrument (17-km resolution) aboard the Terra satellite were compared with final retrievals of AOD (532 nm) from the HSRL (6-km resolution, 550 nm) aboard the King Air B-200. Comparisons were conducted on 7, 12 and 13 March 2006, at which time the King Air B-200 flight intersected the overpass of the Terra satellite. AOD was derived from the HSRL measurements by integrating the aerosol extinction profiles between 0.1 km and 7 km.

3.4 Point selection algorithms

Aerosol optical depth data in Hierarchical Data Format (HDF) from each instrument were imported into MATLAB (version 7.4). To compare data sets, a point selection algorithm was developed to locate MODIS points within 7 km and between one and two hours of the HSRL flight path. This algorithm provided us with only the most relevant data points for our study, thereby enabling a near direct analysis of the MODIS data with the HSRL data.

Data points obtained using the point selection algorithm also were compared to preliminary forecasts from the WRF-Chem. WRF-Chem forecasts provide the capability of simulating chemistry and aerosol concerntrations from mesoscale to synoptic scale. The WRF-Chem forecasts (12-km horizontal resolution nested within 60-km resolution) were analyzed to determine AOD (532 nm) at each coincidence of HSRL and MODIS data. Coincident data points of HSRL, MODIS, and WRF-Chem were imported into a spreadsheet to perform statistical analysis.

3.5 FSU and HYSPLIT Trajectory Comparison

Florida State University's (FSU) trajectory research, which uses in situ u, v, and w wind components collected aboard the DC-8 and C-130 aircrafts, was used to assess the dependability of HYSPLIT. Florida State University campaign flight dates were available for 15 days in March 2006. The altitude and location of the flight path initialization point were inputted into the FSU trajectory calculator and the HYSPLIT model to produce 72-hour forecasts of air particle trajectories. HYSPLIT runs were initialized at 12, 18, and 21 UTC for each day studied.

4. RESULTS

4.1 *Houston Ozonesondes compared to STEM and TES*

For March 2006, STEM ozone concentrations plotted with ozonesonde data showed a correlation coefficient of 0.62 with a sample size of 17 (Figure 1). On 7 and 23 March, the average column values from TES were inconsistent with the average column values from the ozonesondes. The ozone concentrations, as given by ozonesondes, were 234 ppbv over a 21.3-km column and 1360 ppbv over a 29.3-km column. The TES measurements for those days were 231 ppbv and 1800 ppbv respectively. Comparing data from TES and the ozonesondes, percent error values for 7 and 23 March 2006 were 1.3% and 24% respectively.

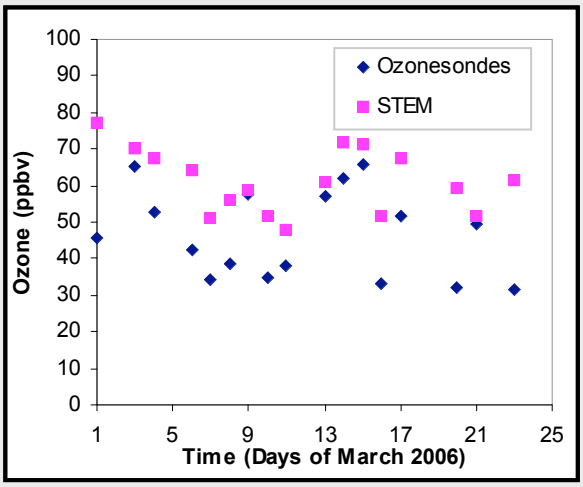

Figure 1: Time Averaged 1km STEM and Ozonesonde Analysis for March 2006

4.2 STEM tropospheric ozone results

For the two compounds investigated (O_3 and NO_2, the latter of which is a precursor to NO_x which itself is a precursor to tropospheric 0_3), Mexico City concentrations were consistently and significantly higher (by more than 300% in the case of ozone) than Houston concentrations. STEM results for March 2006 indicate that Mexico City has an average ozone concentration of 171 ppbv with a standard deviation of 97 ppbv. Houston has an average ozone concentration of 54 ppbv with a standard deviation of 11 ppbv. According to STEM predictions, Mexico City has an average NO_2 concentration of 32.5 ppbv with a standard deviation of 20 ppbv. Houston has an average ozone concentration of 4.6 ppbv with a standard deviation of 3.4 ppbv.

Mexico City and Houston ozone results strongly suggest an increase in O_3 concentration at 18 and 21 UTC. For Mexico City, the concentrations of ozone at 18 and 21 UTC are approximately equal and always higher than the 06 or 12 UTC concentrations (Figure 2).

For Houston, mid-day to late–day average concentrations were higher than 06 and 12 UTC average concentrations (Figure 3). In both locations, the 06 UTC O_3 average concentrations are higher than the 12 UTC average concentrations.

Nitrogen dioxide results for Mexico City and Houston suggest that NO_2 concentrations are lower, on average, during the afternoon hours. Concentrations at 18 and 21 UTC (18 and 00 UTC for Houston) were consistently the lowest of the four data acquisition times. Consequently, 06 and 12 UTC concentrations were highest in both areas of interest (Figures 4 and 5).

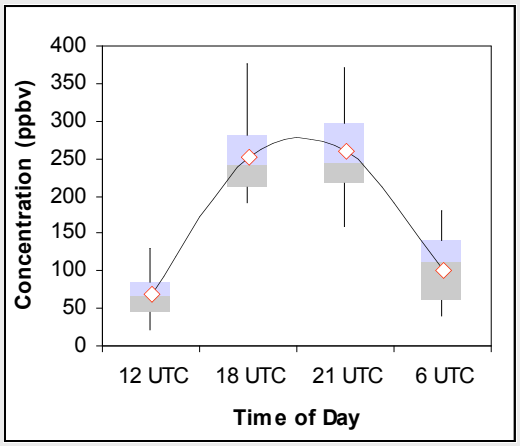

Figure 2: STEM Predicted Tropospheric Ozone Concentrations in Mexico City for March 2006

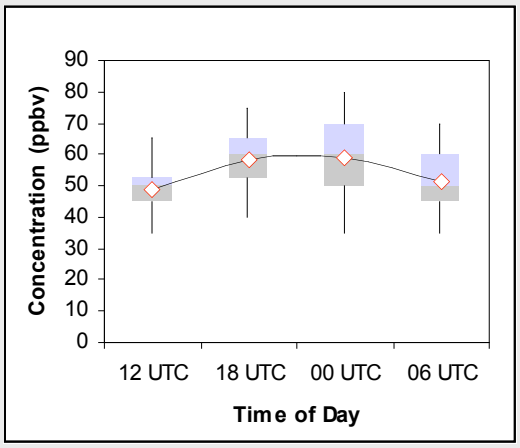

Figure 3: STEM Predicted Tropospheric Ozone Concentrations in Houston, TX for March 2006

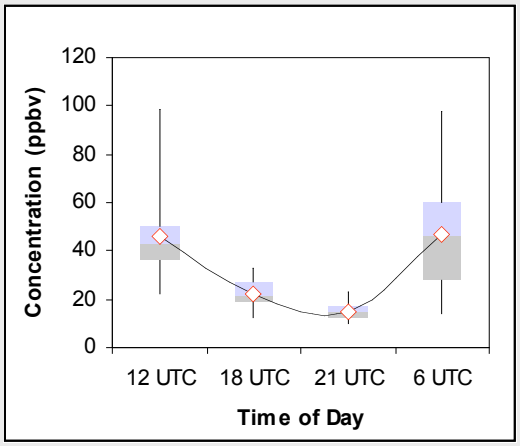

Figure 4: STEM Predicted Nitrogen Dioxide Concentrations in Mexico City for March 2006

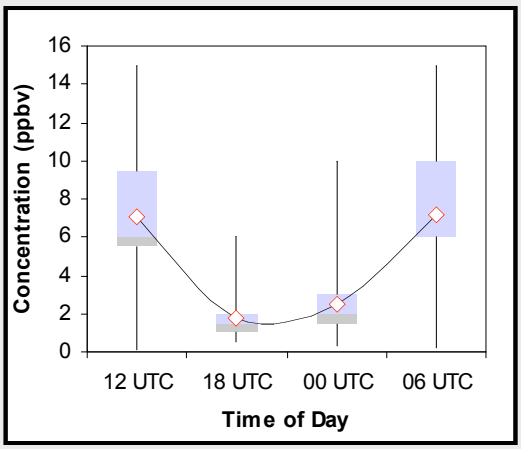

Figure 5: STEM Predicted Nitrogen Dioxide Concentrations in Houston, TX for March 2006

4.3 *Correlation analysis of MODIS with HSRL*

On 7 March, 52 coincident MODIS and HSRL points fell within 7 km of each other between 17.85 and 20.18 UTC (Figure 6). Given the sample size, the MODIS AOD and HSRL AOD were highly correlated with an R-value of 0.87. On 12 March, 34 coincident MODIS and HSRL points fell within 7 km of each other between 16.76 and 18.86 UTC. MODIS AOD and HSRL AOD were correlated with an R-value of 0.74. On 13 March, 74 coincident MODIS and HSRL points fell within 7 km of each other between 17.16 and 19.67 UTC. MODIS AOD and HSRL AOD were moderately correlated with an R-value of 0.53 (Table 1).

4.4 *Correlation analysis of MODIS and HSRL with WRF-Chem*

On 7 March, with a sample size of 20, MODIS AOD showed a correlation of 0.34 with WRF-Chem, and HSRL AOD showed a correlation of 0.57 with WRF-Chem using a sample size of 148 (Figures 7 and 8). On 8 March, HSRL showed a correlation of 0.46 with WRF-Chem using a sample size of 87. With a sample size of 235 on 9 March, HSRL showed a correlation of 0.58 with WRF-Chem. On 10 March, HSRL showed a correlation of 0.64 with WRF-Chem using a sample size of 56. On 12 March, with a sample size of 33, MODIS AOD showed a correlation of 0.23 with WRF-Chem. HSRL AOD showed a correlation of 0.84 with WRF-Chem using a sample size of 110. On 13 March, with a sample size of 43, MODIS AOD correlated poorly (R-value of 0.082) with WRF-Chem, and HSRL AOD showed a correlation of 0.72 with WRF-Chem using a sample size of 110 (Table 1).

Flight Day	Sample Size for HSRL & MODIS	R-value for HSRL & MODIS	Sample Size for WRF-Chem & HSRL	R-value for WRF-Chem & HSRL	Sample Size for WRF-Chem & MODIS	R-value for WRF-Chem & MODIS
7-Mar	52	0.87	148	0.57	20	0.34
8-Mar	n/a	n/a	87	0.46	n/a	n/a
9-Mar	n/a	n/a	235	0.58	n/a	n/a
10-Mar	n/a	n/a	56	0.64	n/a	n/a
12-Mar	34	0.74	110	0.84	33	0.23
13-Mar	74	0.53	110	0.72	43	0.08

Table 1: Correlation analyses between HSRL, MODIS, and WRF-Chem for six days in March, 2006

4.5 *FSU and HYSPLIT Trajectory Comparison*

FSU trajectory and HYSPLIT plots showed good spatial and temporal correlation with some days exhibiting exceptional agreement (Figures 9 and 10). On days in which FSU data and HYSPLIT did not correlate well, multiple forward trajectories were run with an initialization interval of 2 to 6 hours to determine if the disagreement was temporally systematic. No consistent pattern of disagreement was discovered from these runs.

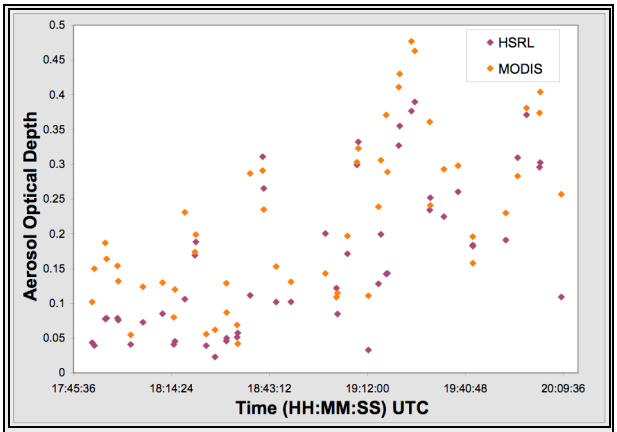

Figure 6: Aerosol Optical Depth Comparison over Mexico City of HSRL vs. MODIS on March 7, 2006

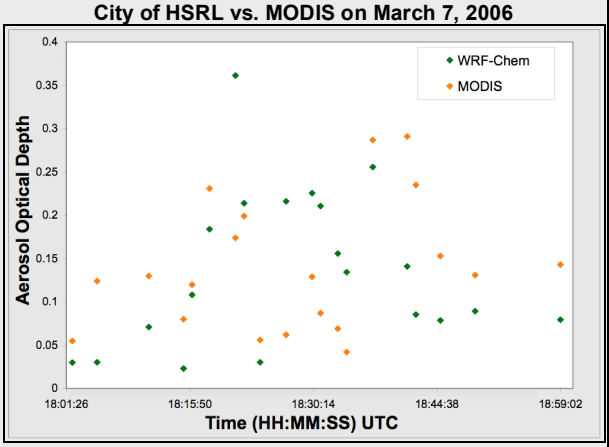

Figure 7: Aerosol Optical Depth Comparison over Mexico City of WRF-Chem vs. MODIS on March 7, 2006

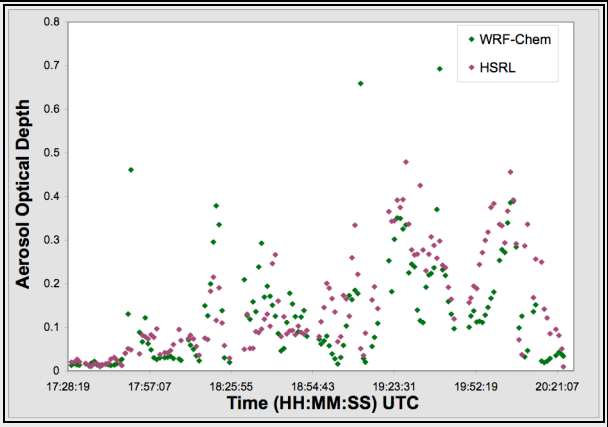

Figure 8: Aerosol Optical Depth Comparison over Mexico City of HSRL vs. WRF-Chem on March 7, 2006

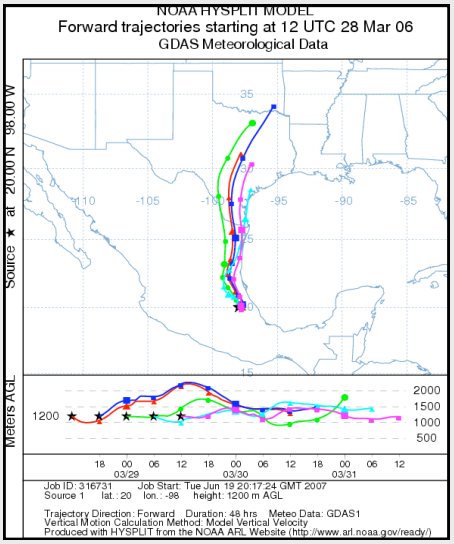

Figure 9: NOAA HYSPLIT modeled aerosol trajectory results started at 12 UTC on 28 March, 2006 in Mexico City

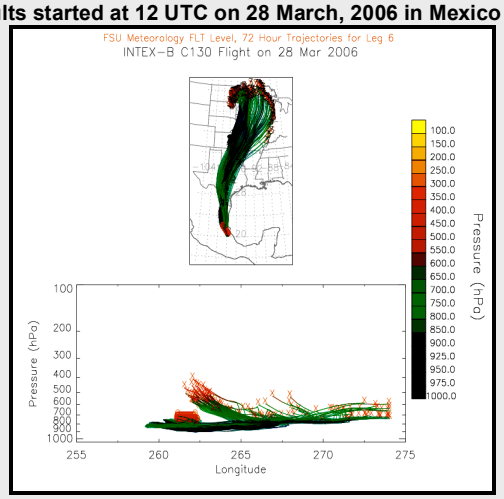

Figure 10: Florida State University 72-hour trajectory results on 28 March, 2006

5. DISCUSSION

5.1 *Houston Ozonesondes compared with STEM and TES*

The final column averaged STEM versus ozonesondes plot showed a statistically significant correlation (0.62), however, STEM ozone values were systematically higher. The variations in the plot might be explained by the time difference between the STEM model runs and the ozonesonde launches.

The first instrument comparison on 7 March 2006 between the Houston ozonesondes and TES was in agreement, but the 23 March measurement showed less agreement. The greater column depth of the measurement on 23 March may have allowed for more sampling error associated with the larger atmospheric column. Additionally, balloon drift (48 and 120 miles on 7 and 23 March respectively) could account for the larger measurement on the 23rd.

5.2 STEM-predicted O_3 and NO_2 concentration

Ozone concentrations were maximized in Mexico City during the local noon and 3:00 p.m. hours (18 and 21 UTC). This result is expected because solar radiation initializes tropospheric ozone formation. It makes sense that NO_2 values would be at a minimum at these same times because NO_2 is one of the precursors to the formation of tropospheric ozone. Nitrogen dioxide levels are higher in the midnight to early-morning hours, and then decrease throughout the day as the solar radiation drives photolysis.

5.3/5.4 MODIS and HSRL with WRF-Chem comparisons

The HSRL and MODIS instruments correlated well on two of the three days. The inconsistencies between the three-way comparisons may have arisen from the WRF-Chem simulations. When WRF-Chem correlated well with HSRL, there was poor correlation between WRF-Chem and MODIS and vice versa. Inconsistencies may have arisen from meteorological or resolution differences.

5.5 FSU and HYSPLIT Trajectory Comparison

From the analysis results, it appears that the HYSPLIT model systematically underestimates particle travel distances relative to the FSU trajectory model. The HYSPLIT model still retains the general trajectory orientation of the FSU results however.

6. CONCLUSION

In order to provide valid results for the scientific study of aerosols and atmospheric chemicals, it is essential that model and instrument observations be compared to provide the highest possible level of accuracy. Using aerosol data observation sources, we were successful in substantiating aerosol models with

regard to concentration and distribution over the study region. Additionally, increasing concerns over the rising threat of tropospheric ozone create an imminent need for future in how to limit the NO_2 production in major cities like Mexico City and Houston.. Forthcoming data from The Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observations (CALIPSO) satellite will provide an enhanced view of vertical AOD distributions, allowing further insight into the distribution and properties of tropospheric chemicals. Further comparisons between HSRL and WRF-Chem will provide insights into model verification of AOD. Finally, though we demonstrated the utility of HYSPLIT, we are inconclusive on the reasons of varying its varying accuracy. A much more in depth study of HYSPLIT is needed to determine the cause of prediction errors, whether they be synoptic related or otherwise. Doing so will allow for an accurate study of how a region's poor air quality can impact another region downwind.

7. ACKNOWLEDGMENTS

We thank the INTEX-B team for the HSRL data and invaluable advice. We thank Dr. Margaret Pippin for assistance in our ozone analysis. Dr. Henry Fuelberg and Jeremy Halland were instrumental in obtaining FSU trajectory data, and we thank Dr. Gary Morris for his aid in obtaining ozonesonde data from Valparaiso and Rice Universities. We thank Dr. Youhua Tang from the University of Iowa for assistance with the STEM analysis, and Dr. Jerome Fast, from Pacific Northwest National Laboratory (PNNL), for help in obtaining WRF-Chem model output. We would like to extend a special thanks to Mike Ruiz, Amber Richards, Diana Laura, Peter Thomas, Jonathan Gleason, Tracey Silcox, and Lindsay Rogers at NASA DEVELOP.

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