

Simulate PM10 Transport from Agricultural Tilling Operations Using Hysplit4

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Abstract Particulate matter (PM) of aerodynamic diameter less than or equal to 10 microns, PM10, is regulated by the U.S. Environmental Protection Agency (EPA) as part of the National Ambient Air Quality Standards (NAAQS). PM10 emitted from agriculture field operations (e.g., disking, listing, leveling, planting, harvesting) can be dispersed downwind in the far-field (i.e., > 1 km). This paper reports on the calibration and evaluation of the Hysplit4 (Hybrid Single-Particle Lagrangian Integrated Trajectory) model to simulate regional dust dispersion from a disking operation. Disking operations in a cotton field at Las Cruces, NM, were conducted, and boundary layer PM10 concentrations were sampled using a Dustrack™ sampler on an airplane flown at altitudes between 200 m and 550 m and downwind several kilometers. Based on the measured data, the model parameters of released particle number, grid size, and particle release height were calibrated. Using NAM12km meteorological data with vertical profiles, the model is capable of reasonably simulating regional PM10 dispersion (the simulated data =1.048×measured data with R²=0.85) when the PM10 was released at

ground level. However, using measured point meteorological data at ground level and the simulated particles were released at ground level, the model error was 90%. The smaller simulated values may be caused by the model's inability to capture the surface layer micrometeorology that transports ground-level dusts to higher altitudes. When using ground measurements of meteorological data, different release heights (50, 100, 150, and 200 m) of the particles were tested, and at the release height of 200 m (top of surface layer), the model performance was the best, the error was 10%, and the R^2 was 0.65.

Keywords: air quality, disking operation, Hysplit4, dynamic model, PM10, pollution

Introduction

Particulate matter (PM) of aerodynamic diameter less than or equal to 10 microns, PM₁₀, is regulated by the U.S. Environmental Protection Agency (EPA) as part of the National Ambient Air Quality Standards (NAAQS). PM₁₀ emitted from agriculture field operations (e.g., disking, listing, leveling, planting, harvesting) is first dispersed downwind in the near-field in high concentration plumes and then dispersed in lower concentrations further downwind in the far-field (i.e., > 1 km) (Hanna et al., 1982). A near-field dynamic model to estimate PM₁₀ dispersion was developed and validated (Wang et al., 2008 and 2009). This model can be used to estimate the PM₁₀ concentration for people working and living immediately downwind of the agriculture field operation (0 to 3 km). A far-field regional model is needed to estimate the PM₁₀

dispersion from agricultural operations for people working and living 3 to 50km down wind. .

Most pollutant dispersion models can be broadly classified as steady-state or dynamic. Steady-state models assume that the environmental conditions (e.g., wind direction and speed and atmospheric stability) are fixed during a long simulation period (e.g., over 1 hour). Steady-state models can be used for industrial pollutant dispersions (e.g., smoke stack dispersion) or other steady-state environments. The regulatory air-quality models (Fugitive Dust Model, FDM; Industrial Source Complex Model, ISC3) at EPA are steady-state models that follow a Gaussian distribution to simulate dispersion (<http://www.weblakes.com/lakeepa1.html>). Each simulation time period is over 1 hour. But with these long mixing times it is difficult to define a single pollutant plume because the material from a specific source becomes well mixed throughout the boundary layer in one time step.

Dynamic models simulate pollutant dispersion using dynamic environmental conditions. The simulation period can be less than 1 minute. For example, the Hysplit4 (Hybrid Single-Particle Lagrangian Integrated Trajectory) model has a minimum time step of 1 minute (Draxler and Hess, 1997). Hysplit4 is more complex than the steady-state models and is more appropriate for PM10 dispersion simulations from agricultural operations. However, Hysplit4 assumes a constant wind speed and turbulence variance in the vertical direction when using user entered data. Although this may be true in the mixing layer, the wind speed and variance profiles in the vertical direction in the surface layer changes

with height. Further, the model grid size and released particle number will affect the model performance. Hysplit4 can also be driven with gridded forecast meteorological data. For example, the forecast data NAM12km has a vertical profile (25-50 m vertical intervals) from 0 m to 1000 m heights with 12 km horizontal resolution and a 3 hour frequency. The objective of this study was to calibrate and evaluate Hysplit4 for the regional PM10 dispersion simulations from agricultural field operations and also compare the use of ground measured meteorological data with NAM12km forecast data respectively.

Materials and Methods

Hysplit4 Model Description

The Hysplit4 model can be adapted for agricultural operation PM10 transport. Hysplit4 was developed by the National Oceanic and Atmospheric Administration (NOAA) (Draxler and Hess, 1997). Hysplit4 for particle sources is based on a Lagrangian model system. The advection of particles is computed from the average of the three-dimensional velocity vectors for the initial-position, $P(t)$ at time t , and the first-guess position, $P'(t + \Delta t)$ at time $t + \Delta t$. The velocity vectors, V , are linearly interpolated in both space and time. The first guess position is

$$P'(t + \Delta t) = P(t) + V(P,t) \Delta t \quad (1)$$

and the final position is

$$P(t + \Delta t) = P(t) + 0.5 [V(P, t) + V(P', t + \Delta t)] \Delta t \quad (2)$$

The source is simulated by releasing particles over the duration of the release. In addition to the advective motion of each particle, a random component to the motion is added at each time step (Δt) according to the atmospheric turbulence at that time. In this way, a cluster of particles released at the same point will expand in space and time, simulating the dispersive nature of the atmosphere.

Particle Dispersion

The particle dispersion equations are formulated in terms of the turbulent velocity components. In the particle implementation of the model, the dispersion process is represented by adding a turbulent component to the mean velocity obtained from the meteorological data. The particle model can be applied in the vertical, the horizontal, or both directions. The specific approach used follows the one described by Fay et al. (1995) and Draxler and Hess (1997).

After computation of the new position at a time step due to the mean advection of the wind, a turbulent component is added to the mean particle positions (X, Z),

$$X_{\text{final}}(t+\Delta t) = X_{\text{mean}}(t+\Delta t) + U'(t+\Delta t) \Delta t, \quad (3)$$

$$Z_{\text{final}}(t+\Delta t) = Z_{\text{mean}}(t+\Delta t) + W'(t+\Delta t) \Delta t, \quad (4)$$

while the turbulent velocity components are in m s^{-1} .

The contribution of the turbulent wind components (U' - horizontal, W' - vertical) are added to the "mean" position (due only to the mean flow) to give a final position from which the advection at the next time step is computed. The variable Δt is the time step, which is a function of the Lagrangian time scale.

Deposition

The deposition from dry removal processes is expressed as:

$$D_{\text{dry}} = m \{ 1 - \exp[-\Delta t (\beta_{\text{dry}})] \} \quad (5)$$

where m is the pollutant mass. The pollutant mass is then reduced by the deposition amount. The dry deposition coefficient (β_{dry}) is calculated as a function of particle settling speed and atmospheric data (Draxler and Hess, 1997).

Hysplit4 Model Inputs

User Entered Meteorological Data and Source Strength

The User Entered Meteorological Data can have one-minute micrometeorological inputs (one spatial point) and includes the following parameters: year, month, date, hour, minute, wind direction ($^{\circ}$), wind speed (m s^{-1}), mixing layer height (m), and Pasqual stability (A-

F). Hysplit4 converts the User Entered data to NOAA Air Resources Laboratory (ARL) packed meteorological data format with 1 km resolution.

In addition, the source strength (mg hr^{-1}) needs to be known to output the absolute concentration. The source strength data (a constant $3,628,800 \text{ mg hr}^{-1}$) from our field study in Wang et al. (2010) were used for the simulations in this study.

NAM 12 KM Meteorological Input

The other type of meteorological data inputs for Hysplit4 is forecast data. The NAM12km forecast data has a vertical profile with data points every 25-50 m from ground level to 1000 m with 12 km horizontal resolution and a 3 hour frequency. The data at and above 50 m includes wind speed and direction, air temperature, relative humidity and total kinetic energy. The surface layer data includes mean sea level pressure, 3-hour accumulated precipitation, 3-hour accumulated convective precipitation, 2 meter temperature, 2 meter relative humidity, 10 meter wind speed, surface pressure, latent heat net flux, sensible heat net flux, friction velocity, surface roughness, downward short wave radiation flux, and surface height.

Hysplit4 Model Output

The model can output the 1-m or larger spatial resolution concentration (mg m^{-3}) at the defined grids with a 1-minute frequency.

Model Parameter Calibration

The model parameters must be calibrated to fit to the agricultural operation (disking operation in this study). The calibrated parameters include the released particle number, grid sizes, and the particle release height. When calibrating one parameter, the other parameters were fixed as: released particle number, 25,000; horizontal grid sizes, 300 m by 300 m; vertical grid size, 50 m; and release height, 5 m. The User Entered Data (ground measured meteorological data) was used for the calibration. All simulations were for the height layers between 200 and 550 m.

The default released particle number in the model was 2,500. To test if 2,500 particles are enough for the simulation, released particle numbers of 2,500, 25,000, and 100,000 were used to simulate PM10 dispersion from disking operations. Linear regression between two groups of simulations (between 2,500 and 25,000, 25,000 and 100,000) was conducted, and the slope and the r^2 values were obtained when the intercept was set to 0. If the slope is above 0.95 and below 1.05 with high r^2 (> 90%) in a group, then the simulations are significantly the same between the two released numbers' group.

Because the horizontal and vertical space grid sizes can affect the outputs (the smaller the grid size, the larger the outputs), different space grid sizes were tested. Because the measured horizontal mean wind speed was 3.4 m s^{-1} , the horizontal grid size should be larger than the value of wind speed multiplied by the time step (one minute), i.e., should be larger than 217 m. The horizontal grid sizes of 200, 300, 500, 1,000, and 2,000 m were tested for simulations at 175 and 600 m altitudes. The regression slope (intercept was set to 0) of outputs at each two-neighbor grid sizes was calculated, i.e., 200 and 300 m, 300

and 500 m, 500 and 1,000 m, and 1,000 and 2,000 m. The first slope that was greater than 0.98 was found, and that corresponding grid size was chosen for the model.

During the field experiments (see *Experiments* section), the airplane's sampling height varied within 50 m in each height layer. Therefore, the vertical grid size was first set to 50 m. The simulations between 50 and 100 m vertical grid sizes were compared to check for significant difference.

When "User Entered Data" was employed, the particle release height could affect the model simulation, especially since the particles were from the ground level and the model may not lift the particles to a higher altitude because the surface layer meteorological simulation may not be appropriate. Therefore, the source height was raised to 5, 100, 150, and 200 m. The simulations were compared with the measured PM10 data, and the best release height was chosen.

Field Experiments

To calibrate and evaluate this model, field experiments were conducted at the Leyendecker Plant Science Research Center at New Mexico State University, Las Cruces, NM, on April 1, 2008 (32° 11' 50.19" N, 106° 44' 18.76" W, elev. 1,173 m). Figure 1 shows maps of the experimental area. A tractor was continuously working in a cotton field (200 x 100 m, yellow area in Figure 1) and disking was operated from 11:13 AM to 13:13 PM Mountain Daylight Saving Time . The figure shows the airplane and tractor locations at 1-second intervals; the locations were recorded by a GPS sensor (010-00321-

00 GPS 18 Deluxe USB Sensor for Laptops, Garmin, Olathe, KS) and a laptop to record 1-second position data, including date, time, altitude, and location as longitude and latitude. A Cessna airplane flew into the operating area at an altitude between 200 and 550 m and sampled PM10 concentrations during the operation. An aerosol monitor (Model 8520, TSI, Inc., Shoreview, MN) was mounted on the airplane to sample PM10 at a flow rate of 1.7 L/min at 1-second intervals. The sampler was factory calibrated, and flow rate was calibrated (1.7 L/min) and the sampler was zeroed in the field prior to the experiments. Two sonic sensors (CSAT3, Campbell Scientific, Logan, UT) were installed in the field to measure the wind speed and direction and turbulence at 1.5 and 9 m heights. The wind data at 9 m was used for the model inputs (User Entered data). Table 2 shows the average meteorological data during the experiments.

Particle Size Distribution

The PM10 consists of different particulate sizes. Different size groups have different mass percentages. The particle size distribution used the data measured in 2005 (Holmén et al., 2007; Wang et al., 2008) in the same field as our cotton disking operations. In the model simulations, the particle sizes were divided into 7 groups as inputs (Table 1).

Outlier Removal

The measured concentration at each 50 m height layer (200 to 550 m) was processed and the mean and the standard deviation were obtained. Then, the outliers were defined as the values out of the range of mean \pm 3 standard deviations. All the outliers were removed from the raw data before other data processing.

Background Removal

After the outlier removal, the concentration data from 20 minutes before the disking operation was started were separated as the background data. The average (0.0048 mg m^{-3}) of the data was used as the background (the standard deviation was 0.0034 mg m^{-3}), i.e., the other measured data removed the background value before comparing with the model simulations.

Simulations

After the model calibration, the model was run for heights from 200 to 550 m every 50 m using the ground measured wind data and NAM12 km data (20080401_nam12) respectively and then the simulated data was compared with the measured concentration data. When the model was run for NAM12 km data, the particle release height was at 5 m, while for measured ground meteorological inputs, the model used a calibrated release height. In addition, the model used other calibrated parameters (release particle number=25,000, horizontal grid size=300 m, and vertical grid size =50m) for all the simulations. All the data outputs were at 1-minute frequency.

The average values at each height layer at the corresponding time and spatial area of the simulations and the observations were compared using linear regression between the observations and the simulations. The slope and the R^2 values were obtained when the intercept was set to 0.

Results

Model Parameter Calibration

Released Particle Number

The slope of the linear regression for the simulations of between 2,500 and 25,000 released particles was 1.05 and R^2 was 0.56; the slope of the linear regression for the simulations of between 25,000 and 100,000 released particles was 0.96 and R^2 was 0.90. Consequently, 25,000 released particles is sufficient and the model simulations will not be improved by more than 4% ($1-0.96$) with increased released particle number. Furthermore, increasing the particle number increases the simulation time for the model to run.

Grid Size

The linear regression slope of simulations vs measured PM10 concentration when the released particle number was 25,000, the vertical grid size was 50 m, and the particle release height 200 m was less than 0.5, when the horizontal grid size was 200 and 300 m. The slope of the linear regression increased to 0.98 when the grid size was increased to 300 and 500 m and then the slope decreased to 0.92 and 0.73 when the grid size increased to between that of 500 m and 1000 m, and 1000 m and 2,000 m, respectively (Table 3). Therefore, 300 m was chosen as the horizontal simulation grid size.

The airplane sampling heights varied by about 50 m due to large eddy turbulence effects on the small plane. Therefore a 50 m vertical grid was chosen for the model. The regression slopes of the simulations between the 50 and 100 m vertical grid sizes were greater than 0.9 and the R^2 was greater than 0.9.

Particle release height

The linear regression slopes between the simulations and the concentration data when the intercept was 0 and using the ground measured meteorological data as inputs, increased from 0.1 to 1.1 when the release height increased from 5 to 200 m. Simulations at 200 m release height showed the closest fit to the measured data (slope = 1.1, $R^2 = 0.65$), (The R^2 ranged from 0.59 to 0.71 for different release heights (Figure 2)).

The lower accuracy at lower release heights may have been due to the assumption in the model of a constant wind speed and turbulence variance in the vertical direction when using User Entered data. Although it may be true in the mixing layer, the wind speed and variance profiles in the vertical direction in the surface layer changes with height. Without these changes, especially the smaller turbulence variance at the ground level, the model may have brought less PM10 from ground level to the mixing layer. When using User Entered data (ground measurement), raising the source to an appropriate higher height (200 m) can improve the model performance.

Evaluation of simulations using NAM12 km data

Using the 12 km gridded forecast data NAM12 km Figure 3 shows sample simulated PM10 concentration outputs (mg m^{-3}) from Hysplit4 at 200 and 550 m heights at 30, 60, and 90 minutes after the disking operation started. As expected, the plume size increased with time. Thirty minutes after the disking operation started, the simulated plume had spread 6.3 km in the mean wind direction and maximum 2.1 km in the crosswind direction. After 60 minutes, the simulated plume had spread to 16.9 km in the mean wind

direction and maximum 7.3 km in the crosswind direction. After 90 minutes, the plume had spread to 22.5 km in the mean wind direction and maximum 11.5 km in the crosswind direction.

Figure 4 shows the comparison of the model simulation to the observation at different heights using NAM12 km weather data. Generally, the measured and the simulated concentrations decrease with height. The linear regression shows that the simulated=1.048×measured with R^2 0.85. Therefore, the Hysplit4 model is capable of simulating regional PM10 dispersion from agricultural tilling operations given appropriate meteorological inputs and calibrated parameters as long as the source strength input is accurate. Because the airplane sampled the concentration at the farthest distance 6 km downwind, the model accuracy further downwind should be tested in the future.

Conclusion

Hysplit4 is capable of simulating regional PM10 dispersion from agricultural tilling operations using appropriate meteorological data inputs and calibrated parameters. The appropriate meteorological data is spatially distributed NAM 12 km meteorological forecast data rather than direct surface measurements.

Compared with the measurements of PM10 from agriculture operations from 200 to 550 m heights, the Hysplit4 model outputs reasonably accurate concentrations in the

downwind area using NAM 12 km meteorological data as input. The regression analysis shows that the simulated data =1.048×measured data with $R^2=0.85$.

On the other hand, if single point meteorological measurement at ground are used as input to Hysplit4 as “User Entered Data”, Hysplit4 does not accurately simulate the PM10 dispersion from a field disking operation because the model does not consider the vertical change of the surface layer meteorological parameters and cannot raise the PM10 from the ground level to the mixing layer. In order to use surface measurements of wind to drive the model and obtain reasonable accuracy, it was necessary to raise the source release height to 200 m (to the top of the surface layer).

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Table 1. PM10 particle size distribution in Holmén et al. (2007) and Wang et al. (2008). The settling speeds were calculated by Stoke's Law.

Particle diameter (D_p) range nm	Particle geometric mean diameter used in the model nm	Total weight percentage (particle weight divided by total weight of all particles)	Settling speed $m\ s^{-1}$
$7 \leq D_p < 387$	123.0	0.011	9.5E-07
$387 \leq D_p < 621$	490.2	0.005	1.5E-05
$621 \leq D_p < 960$	772.1	0.015	3.8E-05
$960 \leq D_p < 1,620$	1,247.1	0.154	9.8E-05
$1,620 \leq D_p < 2,420$	2,000.0	0.634	3.0E-04
$2,420 \leq D_p < 6,660$	4,014.6	0.051	1.0E-03
$6,660 \leq D_p < 10,060$	8,185.3	0.130	4.2E-03

Summation

1.0

Table 2. Average atmospheric data for Hysplit4 for simulations in April 1, 2008. Values in parenthesis are standard deviations. Stability 1 represents Pasquill Stability class A, very unstable.

Date	Duration	Wind direction (°)	Wind speed (m/s)	Mixing height (m)	Pasquill stability
April 1	11:13- 13:13	156.5 (30.2)	3.4 (1.0)	1,500 (0)	1(0)

Table 3. Linear regression slope and (R^2) of simulations with different horizontal grid sizes at 200 to 550 m altitudes when regression intercept equaled 0. (Released particle number was 25,000, vertical grid size was 50 m, and particle release height was 200 m.)

grid size (m)	300	500	1,000	2,000
200	0.41(0.19)			
300		0.98(0.7)		
500			0.92 (0.63)	
1,000				0.73 (0.73)

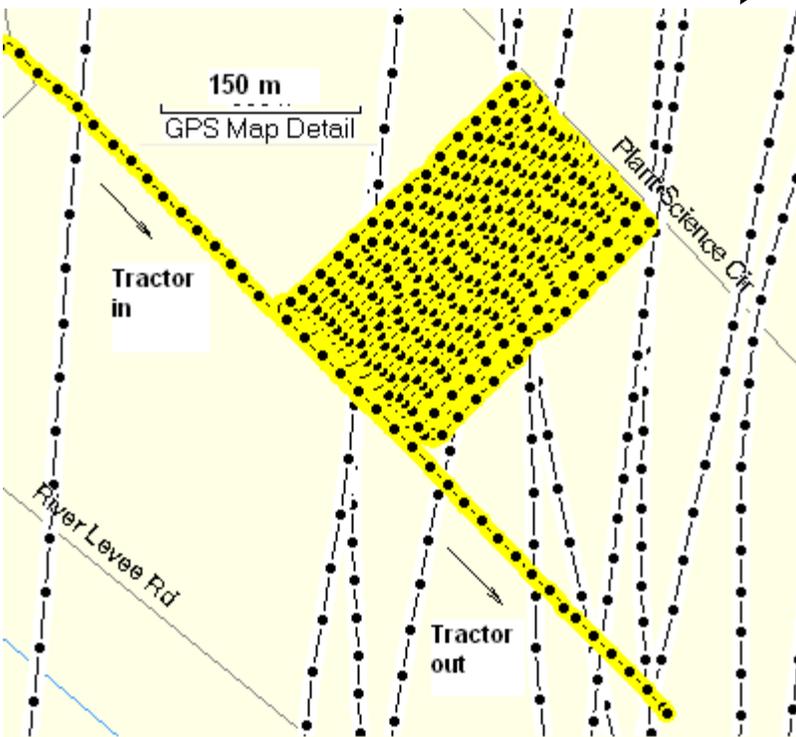
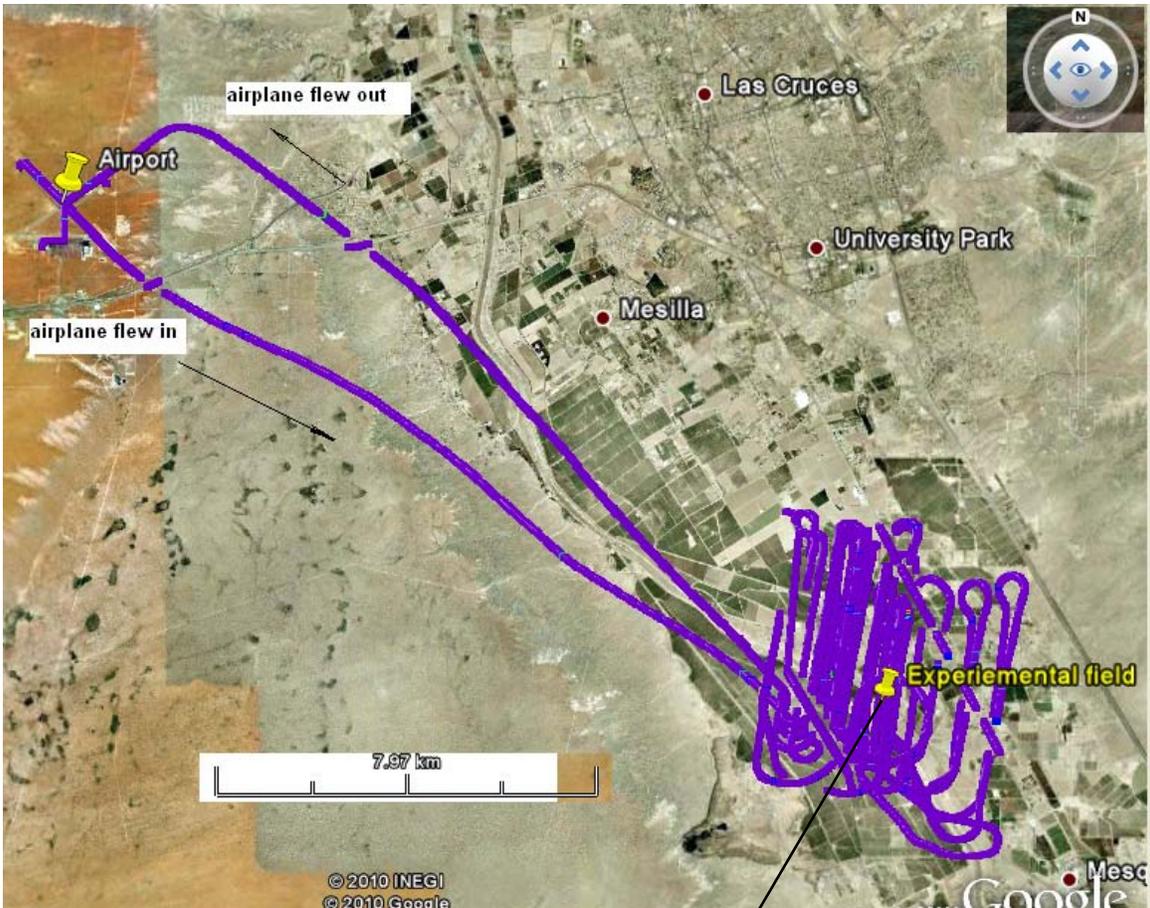


Figure 1. The GPS locations of tractor (bottom graph) and airplane (top) for the disking operation on April 1, 2008.

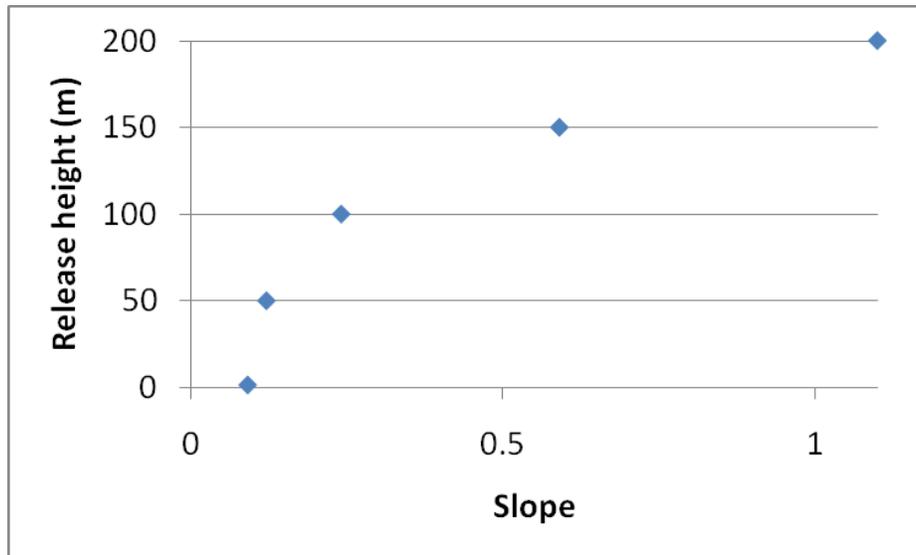
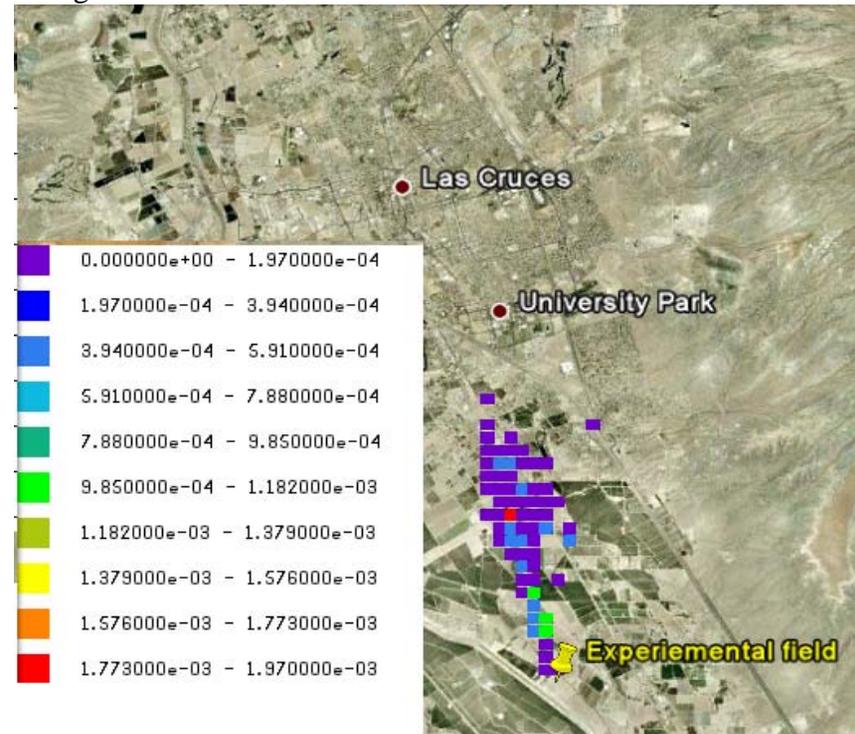
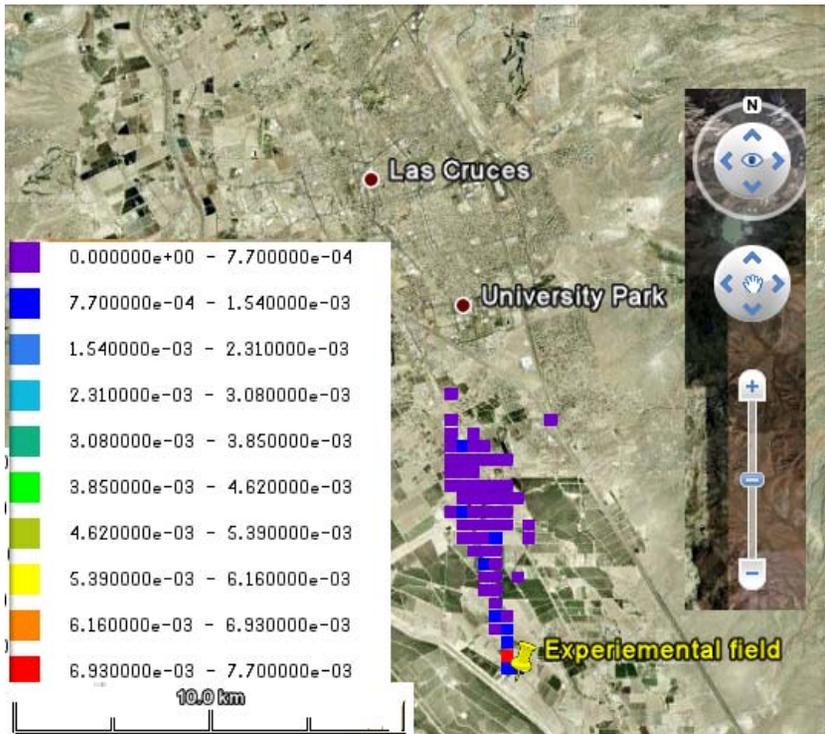


Figure 2. The slope (accuracy index) variation with particle release height using User Entered data (ground measurement). The slope is the linear regression slope of simulation vs observation when observation was the independent variable and intercept was 0. The value of r^2 changes from 0.59 to 0.71 for the different release heights.

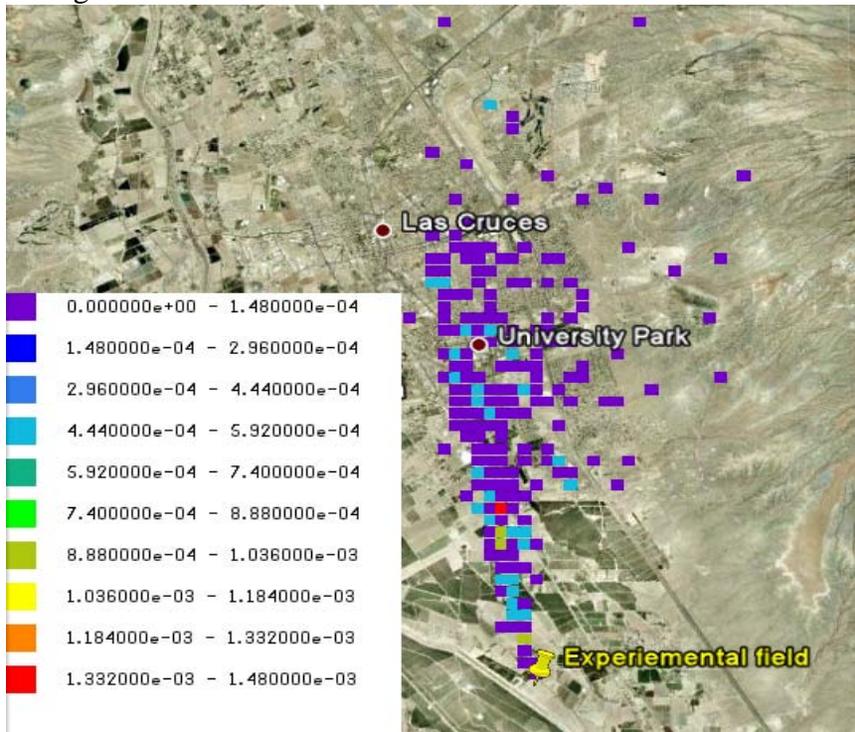
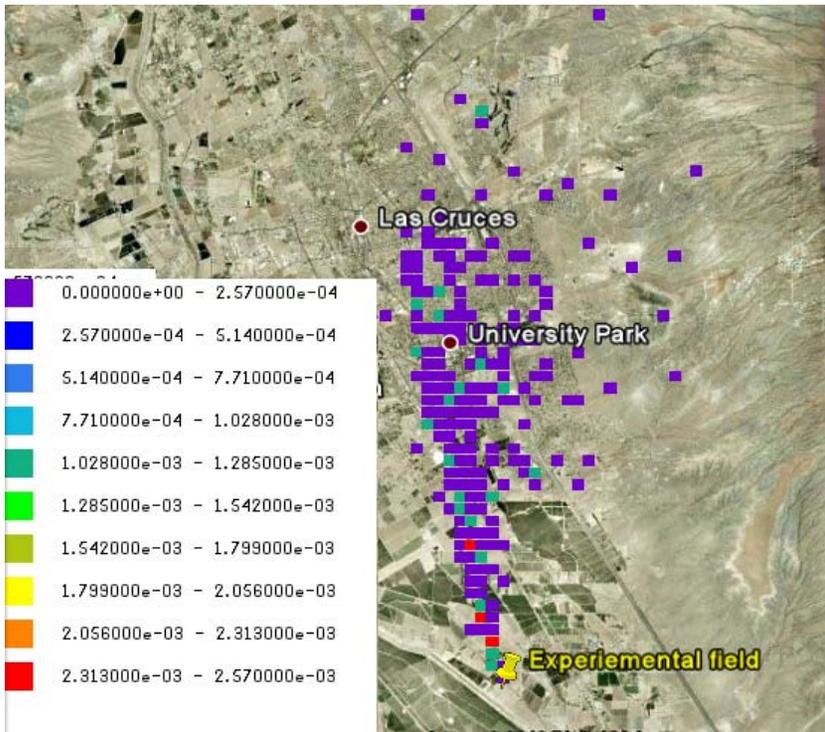
at 200 m height

at 550 m height

30 minutes after disking started



60 minutes after disking started



90 minutes after disking started

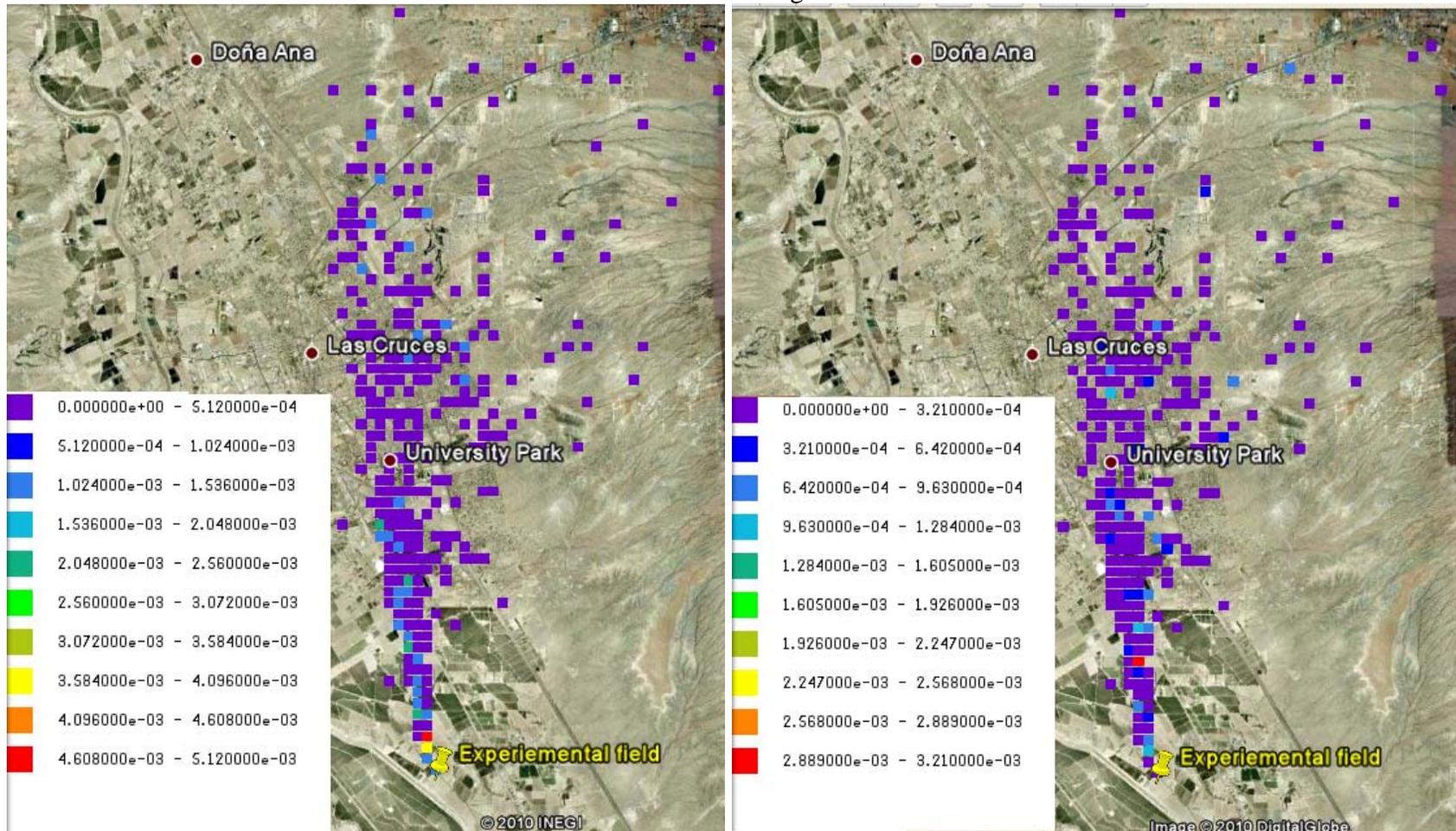


Figure 3. Hysplit4 simulated PM10 concentration (mg m^{-3}) at 200 m (left) and 550 m (right) height at 30 (left), 60 (middle), and 90 (right) minutes after the disking operation started on April 1, 2008.

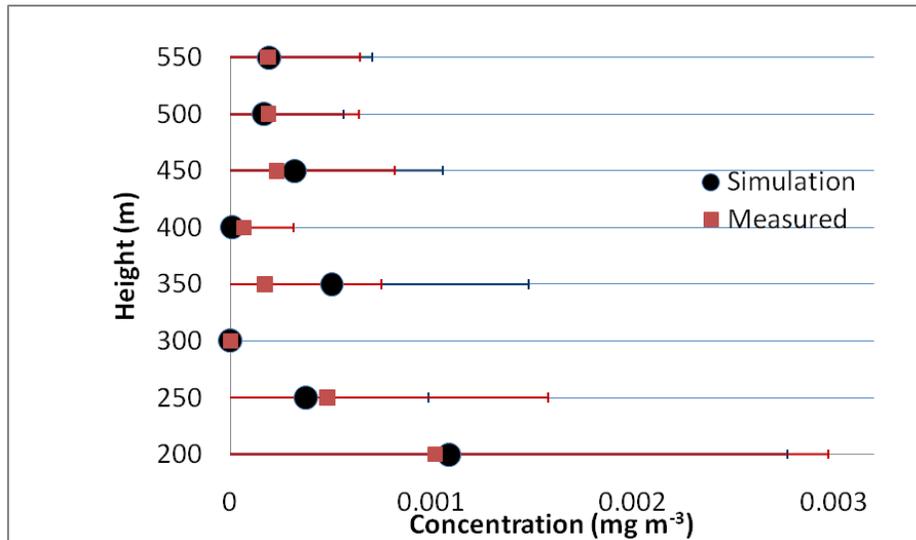


Figure 4. PM10 concentration comparison between observation and simulation at different heights for 11:13 to 13:13 on April 1, 2008. Bars are the standard deviations. The concentration of the simulation at each height was calculated for the downwind plume area that intersected with the concentration of observation. The measured data have the background concentration, 0.0048 mg m^{-3} , subtracted. At 300 and 400 m heights, the simulated and measured data were overlapped and compared at the edge of the plumes; therefore, the concentrations were close to 0.

