PAPER# 3.5

DEVELOPMENT AND VALIDATION OF A LAGRANGIAN MODEL FOR DUST GENERATED BY AGRICULTURAL TILLING

28th Conference on Agricultural and Forest Meteorology

Junming Wang*[1], D. R. Miller[2], A. L. Hiscox[2], and T. W. Sammis[1]

ABSTRACT

Human exposure to dust in and near farm fields is an increasing concern. This paper presents a dynamic lagrangian particle transport and dispersion model which simulates the field-scale dust dispersion from cotton field tilling. The major model inputs are the source strength (g/s, or particle numbers/s), the dynamic wind and turbulence (wind friction velocity, u*), wind direction, and atmospheric stability.. The particle concentrations in the air in 3-D can be obtained at any time. The model was programmed using C++ language, has a user-friendly interface with graphic output (4-D contours, x, y, z, and concentration). Model simulations are verified with remotely measured dust plume concentration and spread obtained by an elastic backscatter lidar. Multidimensional dimensional autocorrelation and cross-correlation analyses are used to quantify the model-lidar comparisons.

Corresponding author address:
(1)JUNMING WANG
New Mexico State University Department of Plant and Environmental Sciences Box 30003 MSC 3Q, Skeen Hall Room, Las Cruces, N.M. 88003-8003, Phone Number: 1-575-6463239, Fax Number: 1-575-6466041, *jwang@ nmsu.edu*

(2)Dept. of Natural Resources Mangament and Engineering, University of Connecticut1376 Storrs Road, U-408,7Storrs, CT 06269

1. INTRODUCTION

Particulate matter (PM) of aerodynamic diameter less than or equal to 10 microns, PM10, is regulated by EPA as part of the National Ambient Air Quality Standard (NAAQS) pollutants. PM10 is directly emitted from a wide range of industrial point sources (power plants, incinerators, cement plants), mobile sources (automobiles and trucks), and non-point sources such as agricultural operations (e.g., land disking, harvesting, cattle ranches) and construction sites. PM10 emissions from agriculture field operations (e.g., disking, listing, leveling, planting, harvesting) is first dispersed downwind in the near-field in high concentration plumes and is then is dispersed in lower concentrations further downwind in the far-field (>1 km). short-event doses. (Hiscox et al., 2007). The theoretical ensemble average is made up of individual events which are widely distributed in their initial path directions and are dynamic on time scales of seconds to minutes. The distance from the source to the boundary between near-field and far-field is dynamic and depends on the wind, turbulence fields and people nearby to be high-density, Only limited attempts to model individual near field dispersion events have been made and the majority of these have been in urban areas (Coirier and Kim 2006 a, b; Flaherty, et al. 2007; Hamel et al., 2006; Haupt et al 2007).

Several near-source unpaved road dust modeling studies have been conducted with steady-state Gaussian models such as the EPA ISCST3, Industrial Source Complex Short Term model (http://www.epa.gov/scram001/dispersion_alt.htm#isc3) (Veranth et al., 2004; Etyemezian et al., 2004; Etyemezian et al., 2003; Chow et al., 1999). Drawbacks to using Gaussian models for modeling near-field dust dispersion from agriculture operations are the model requirements of steady-state environmental conditions and releases from a continuous fixed-location line or point source. Agricultural PM10 sources are not fixed sources and are moving sources because the operation equipment (e.g., tractor, harvester) is traveling continuously in the field. A dust puff will be produced at a new location when the equipment moves to the new location.

Eulerian dynamic models (based on the atmospheric diffusion equation) have also been developed to simulate unpaved road dust dispersion (e.g., Veranth et al., 2004; Etyemezian et al., 2003). These models simulate dust movement better than the steady–state Gaussian models because of the model's dynamic characteristics. However, the application of Eulerian models for estimating scalar transfer by turbulence has been limited by their inability to accurately model the dispersion of material from near-field sources (Van den Hurk and Baldocchi 1990).

Lagrangian models do not suffer from this deficiency since they explicitly consider the diffusion of material in both the near-field and the far-field (Van den Hurk and Baldocchi, 1990). Lagrangian models to simulate gas and particle trajectories in three dimensions from steady-state continuous, fixed point, line and area sources have been reported (e.g., Aylor and Flesch, 2001; Aylor and Ferrandino, 1989; Wilson and Shum, 1992). In these models, particle movements are driven by wind velocities calculated in each time step (∇t) from inputs of mean wind speed, direction, and turbulence statistics. The final particle or puff concentration at a point is calculated as the particle number divided by the local volume. Wang et al (1995) utilized a Lagrangian model to describe the movement of spray aerosols released from a moving aircraft. But to our knowledge, no Lagrangian model has been developed to predict the dynamics and concentrations of individual near-field events during agriculture operations.

The objective of this paper is to report the development and validation of a dynamic field-scale (near-field) model for dust dispersion simulations from an agriculture operation (disking).

2. Methodology

2.1 The simulation model

A computer-run Lagrangian simulation model was developed to simulate the dynamic three dimensional PM10 near-field dust dispersion and concentrations (μg m^{-3}) from agricultural field preparation operations. The model physics follows theory and methods of Aylor and Ferrandino (1989), Wilson and Shum (1992), Wang et al.(1995) and Aylor and Flesh (2001). But the model described here adapts the theory to moving sources and is driven by dynamic, rather than steady-state meteorological inputs. This model was programmed in the c++ computer language and is a user-friendly software package. This model version excludes any particles generated by the farming equipment that are larger than 10 μm.

2.1.1 Inputs and Outputs

The model inputs include: Simulation time period length, t (s). PM10 source strength, Q (μg s^{-1}), measured by Wang et al. (2007) using PM10 samplers, friction velocity, u^* (m s^{-1}), mean wind direction, and Monin-Obukhov Length (L, m) for each 1-second period, measured using sonic anemometers. The model outputs are the 3-D concentration c(X, Y, Z, t) (μg m^{-3}).

2.1.2 Model formulations

Turbulent air flow along a particle trajectory is simulated by the three-dimensional Lagrangian stochastic model. The model follows Wang et al, (1995) and satisfies the Thompson (1987) well-mixed criteria. Since the PM10 particles being modeled are small (<300 μm) the inertia "crossing trajectory" effect is ignored (Casanady, 1963, Sawford and Guest, 1991) and the particles are treated as passive scalars.

After Wilson and Shum (1992) the random flight of each dust particle is simulated as a Markov process in a sequence of short time steps, during each of which the particle moves by:

$$dx = [\bar{u}(z) + u]dt \ ,$$

$$dy = vdt \ ,$$

$$dz = (w - v_S)dt \qquad (1)$$

where $\bar{u}(z)$ (m s^{-1}) is the mean along wind velocity at the present height of the particle, u, v, and w (m s^{-1}) are the along wind, crosswind, and vertical turbulent velocities, respectively, and v_s (m s^{-1}) is the settling velocity of the particle, dt is the time duration of a time step (s).

The velocity fluctuations are formulated as (Wilson et al., 1992):

The particle deposition algorithm follows Aylor and Ferrandino (1989).

2.1.3 Simulation implementation

The tractor movement on the X axis (from origin to the X positive direction or from the X positive direction to origin) is divided into segments. Each segment is 0.5 m and is assumed as an instant puff source. When the tractor moves in a segment, 30,000 particles are released from the particle class with geometric mean diameters 2000 nm.

The wind direction, speed and atmospheric stability are never steady over the entire simulation period, which in this case is the 3 minutes it took for the tractor to traverse the field. Thus we use short-time periods, on the scale of 1.0 second, to input atmospheric data to drive the simulation. One-second averages of u*, wind direction, and L measured by an in-field sonic anemometer are used.

CPU resources are generally limited, therefore we only simulate the flights of the particle class of geometric mean diameter of 2000 nm, with a settling velocity of 0.0003 m s^{-1}, because the final output is the weight-based concentration and the 2000 nm particle has the largest weight proportion in the particle classes. The PM10 particle size distribution, in the simulation shown herein, was measure by Holmén et al. (2007). Particles less than or equal to 10 μm are all small enough and the settling speed is so small that their motion in the atmosphere is essentially the same. Therefore it was necessary to model only one particle size class to simulate the entire PM10 distribution.

2.1.4 Simulated concentrations

In each simulation, the random-walk model tracks each particle until it is deposited on the ground or until the simulation time runs out. For calculating the particle concentration at a point (X, Y, Z) and at time t, a “detection cube” is defined with a side length of 1 m and volume $\nabla V = 1$ m^3. The particle number in the cube at time t is counted and the concentration (μg m^{-3}) is calculated based on the particle density, volume and number.

2.2 Field verification experiments

The model was applied to simulate the 2005 dynamic dust dispersion experiments from disking operations in an irrigated cotton field near Las Cruces, New Mexico described by Holmén et al. (2007) and Hiscox et al. (2007).

A 3-D sonic anemometer (CSAT3, Campbell Scientific Inc, Logan, UT) was located at 1.5 m height at the field edge to measure the 20 Hz wind component velocities (u, v, w). The friction velocity (u_*), Monin-Obukhov Length (L) and wind direction were obtained for each sampling pass and each second.

Dust plume size, shape and movement were measured remotely via the University of Connecticut portable backscatter elastic Lidar at approximately 45 second intervals. The Lidar specifications are listed in Hiscox et al. (2006). The The slices from each scan were combined in Lidar data analysis software to characterize the three dimensional plume on this time scale (Hiscox et al., 2006).

Sampling was conducted during each pass and afterwards for several minutes. At the end of the pass, the tractor stopped at the end of the field and turned off its engine until all sampling was completed and the dust plume generated had moved out of the sampling area. Then another pass across the field was made.

The average source strength Q was 350 $\mu g\ s^{-1}$ for 23 disking passes, determined from measurements of a GT640A sampler (Met One Instruments, Inc., Grants Pass, OR) and a ELPI low pressure, cascade impactor, sampler (Dekati LTD., Finland). The procedures and calculations to determine the source strength are described by Wang, et al. (2008).

3. Results

The model performance was evaluated by comparing the modeled plume characteristics with those measured remotely with the University of Connecticut Elastic Backscatter Lidar. Plume dispersion, plume shape and plume concentrations and locations were compared.

3.1 Plume Dispersion Comparison

Outputs were first compared with the Lidar data by comparing the Lidar measured Gaussian plume dispersion parameters (σ_y, and σ_z) with those calculated from the model run.

The comparisons of σ_y and σ_z were made at 10 m to 50 m, 100 m, and 160 m in the down plume direction. Overall the ratio of simulated σ to measured σ ranged from 0.77 to 1.24. In the horizontal (σ_y), on average, the model underestimated the measured plume dispersion by 21% near the source but was very close at further distances. In the vertical (σ_z), the simulation slightly underestimated the measurements near the source, was nearly equal at 100 m and overestimated by 24% at 160 m away.

3.2 Plume shape comparisons

Figure 1 shows a simulation of the model and the corresponding Lidar measurements for pass 20. It plots (x,y) relative concentrations in horizontal slices through the plume at three heights and demonstrates the spatial patterns of the dust plume. Figure 1 demonstrates similar patterns from the Lidar measurements and the model simulation.

The Lidar measurements show a bend in the plume downwind from the source where the dust plume was oriented in different directions at different distances especially at the 3 m height. The model was able to capture these basic direction meanders due to the input of the short time wind direction fluctuations. However, the model simulations were smoother with less spatial variability than the Lidar observations.

We believe that much of the difference between the observations and the simulations is due to the fact the dynamic wind field was not accurately represented over the whole simulation domain by measurements at one point in the field.

3.3 Statistical comparison of plume concentrations and locations.

In order to quantify the pattern correlation between the simulated and measured concentrations, two-dimensional spatial cross-correlations were calculated after Mayor et al. (2003).

Figure 2A shows the 3 m cross-correlation coefficients which have a peak coefficient of 0.78. This high correlation implies a close spatial pattern similarity between the measured and modeled plumes. Figure 2B and 2C show lower peak correlations, 0.65 at 9 m and 0.44 at 15 m. As discussed before, we believe that the lower similarity at higher heights between measured and modeled concentration patterns is also due to the fact the dynamic wind field was not accurately represented at higher heights by a sonic wind measurement at a single height (1.5 m).

4. Conclusions

The dynamic Lagrangian PM10 transport model presented here is capable of accurately simulating near-field dust dispersion from agriculture field operations. The major model advantage over other existing near-field models is that it can simulate moving sources and plume meander.

5. ACKNOWLEDGEMENTS

This work was supported with funds from the U.S. Department of Agriculture NRI CSREES program under contract 2004-35112-14230, the University of Connecticut, Storrs Agricultural experiment station and the New Mexico State University Agricultural Experiment Station. The authors are grateful to staff at the Agricultural Experiment Station at New Mexico State University for their generous cooperation during the field experiments.

6. REFERENCES

Aylor DE, Ferrendino F.J, 1989. Dispersion of spores released from an elevated line source within a wheat canopy. *Boundary-Layer Meteorol*, 46, 251-273.

Aylor DE and Flesch TK, 2001. Estimating spore release rates using a Lagrangian stochastic simulation model. *J. Appl. Meteorol*, 40,1196-1208.

Campbell GS and Norman JM, 1998. *An introduction to environmental biophysics*. Second edition, Springer.

Chow JC, Watson JG, Green MC, Lowenthal DH, DuBois DW, Kohl SD, Egami, RT, Gillies JA, Rogers CF, Frazier CA and Cates W, 1999. Middle- and Neighborhood-Scale Variations of PM10 Source Contributions in Las Vegas, Nevada; *J. Air & Waste Manage. Assoc*, 49 (6), 641-654.

Coirier WJ and Kim S, 2006a. CFD modeling for urban area contaminant transport and dispersion: Model description and data requirements. Preprints, *Sixth Symp. on the Urban Environment*, Atlanta, GA.

Coirier WJ and Kim S, 2006b: Summary of CFD-Urban results in support of the Madison Square Garden and Urban Dispersion Program field texts. Preprints, *Sixth Symp. on the Urban Environment*, Atlanta, GA, Amer. Meteor. Soc., CD-ROM, J5.5.

Csanady GT, 1963. Turbulent diffusion of heavy particles in the atmosphere. *J. Atmos. Sci*, 20, 201-208.

EPA, 1998. *User's guide for the ams/epa regulatory model – AERMOD*. U.S.Environmental Protection Agency Office of Air Quality Planning and Standards Emissions, Monitoring, and Analysis Division Research Triangle Park, North Carolina 27711. November, 1998.

Etyemezian V, Gillies J, Kuhns H, Nikolic D, Watson J, Veranth J, Labban R, Seshadri G. and Gillette D, 2003. *Field testing and evaluation of dust deposition and removal mechanisms*, Final Report on Western States Air Resources Council, Lake Oswego, OR.

Etyemezian V, Ahonen S, Nikolic D, Gillies J, Kuhns H, Gillette D and Veranth J, 2004. Deposition and Removal of Fugitive Dust in the Arid Southwestern United States: Measurements and Model Results. *Journal of the Air and Waste Management Association*, 54, 1099-1111.

Flaherty JE, Allwine KJ, Brown MJ, Coirier WJ, Ericson SC, Hansen OR, Huber AH, Kim S, Leach, M J, Mirocha, J D, Newsom, RK, Patnaik G and Senocak I, 2007. Evaluation study of building-resolved urban

dispersion models. *7th Symposium on the Urban Environment*, 10-13 September 2007, San Diego, CA.
Hamel D, Chwastek M, Farouk B, Dandekar K and Kam M, 2006. A Computational Fluid Dynamics Approach for Optimization of a Sensor Network. *IEEE International Workshop on Measurement Systems for Homeland Security*, Contraband Detection and Personal Safety Alexandria, VA, USA, 18-19 October 2006.
Haupt SE, Young G, Beyer A and Long K, 2007. Assimilating Sensor Concentration Data into a Dispersion Model in a Meandering Flow Field. *11th GMU Conference on Atmospheric Transport and Diffusion Fairfax*, VA July 10, 2007.
Hiscox AL, Miller DR, Holmén BA, Yang W and Wang J, 2007. Near field dust exposure from cotton field tilling and harvesting. *Atmospheric Environment*, in press.
Holmén BA, Miller DR, Hiscox AL, Yang W, Sammis TW and Bottoms R, 2007. Near-Source Particulate Emissions and Plume Dynamics from Agricultural Field Operations, *Atmospheric Environment*, in press.
Mayor SD, Tripoli GJ, Eloranta EW, 2003. Evaluating Large-Eddy Simulations Using Volume Imaging Lidar Data. *Monthly Weather Review*, pp. 131, 1428–1452.
Sawford BL and Guest FM, 1991. Lagrangian statistical simulation of the turbulent motion of heavy particles. *Boundary-Layer Meteorol*, 54, 147-166.

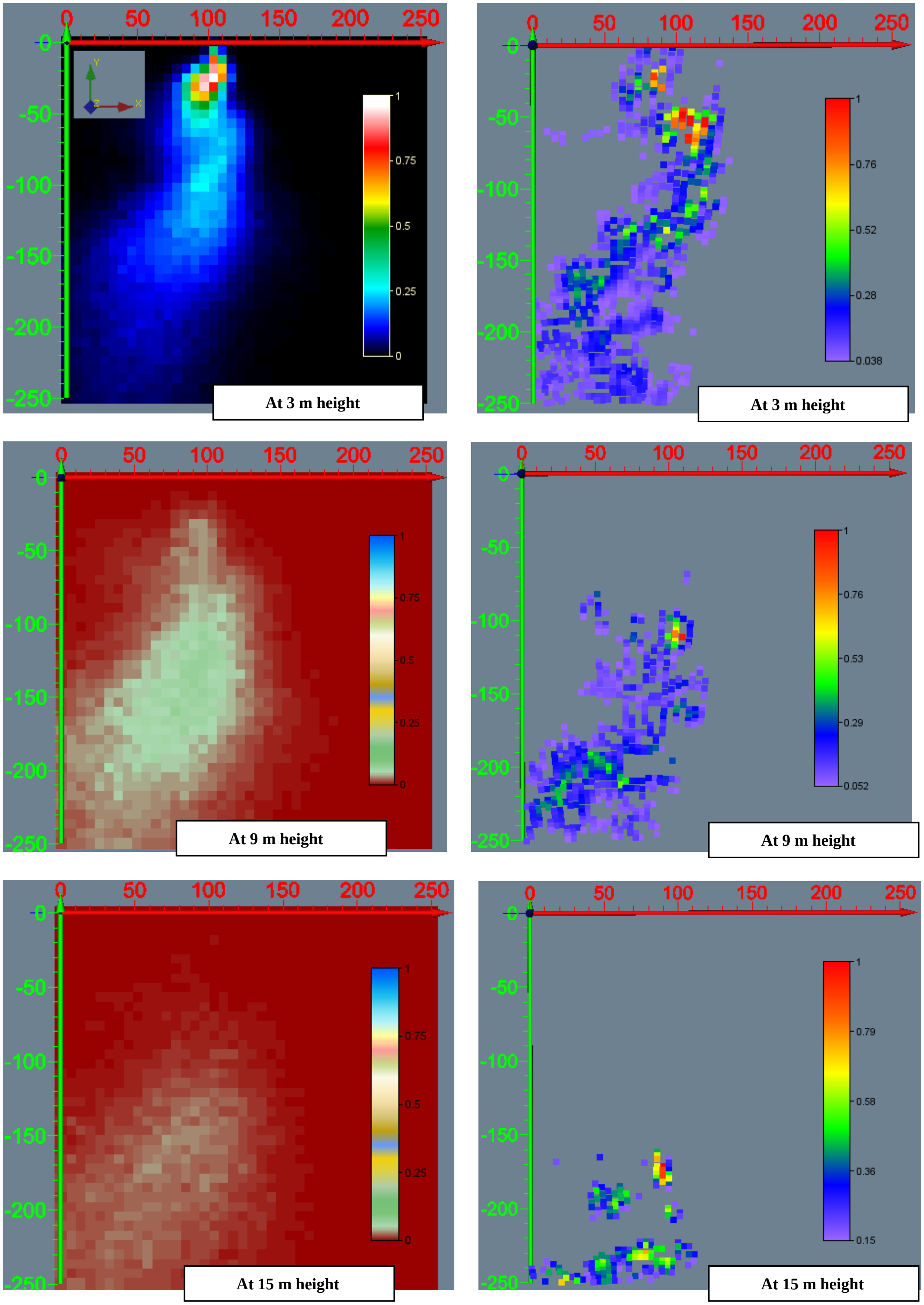
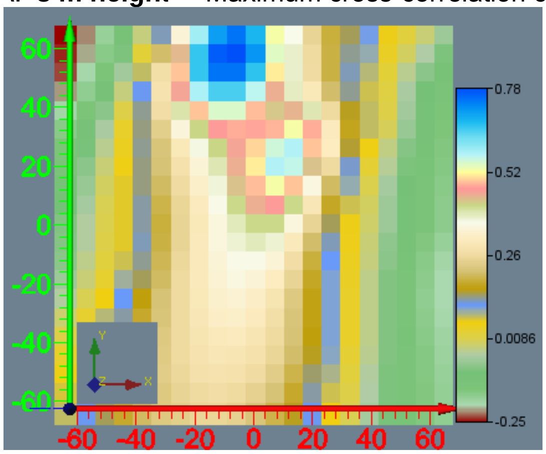
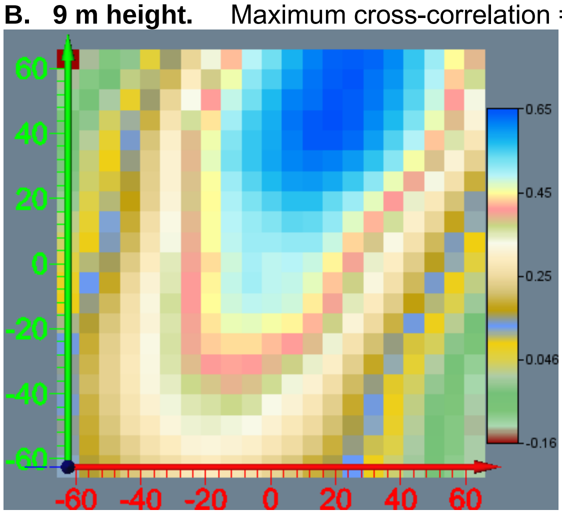


FIGURE 1. The comparison of model simulation (left) and observation (right) of instantaneous normalized dust concentration at different heights from a disking operation (pass 20) at 102 s after tractor started.

A. **3 m height** Maximum cross-correlation coefficient =0.78



B. 9 m height. Maximum cross-correlation =0.65



C. 15 m height. Maximum cross-correlation =0.44

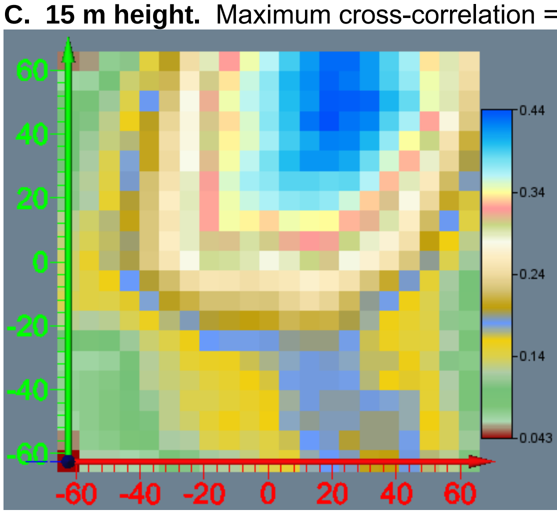


FIGURE 2. Two-dimensional cross correlation between the Lidar measured and the modeled dust concentrations at A) 3 m above the ground, B) 9 m above the ground, and C) 15 m above the ground.