

# 作物農地微氣象層氣懸顆粒分佈

## Micrometeorological Layer/Surface Distribution of Airborne Particles over a Crop Field

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### 摘 要

本文目的為描述作物農地紊流結構及以馬可夫鏈為主之新隨機步行模式以提供一傳輸模式預測農地微氣象層氣懸顆粒分佈。新隨機步行模式考慮對非均質紊流，非零梯度垂直速度之標準偏差，及垂直方向紊流速度之動差偏態作用。文中並討論該模式與其他隨機步行模式比較情形。模式模擬結果顯示紊流速度之動差偏態不僅彌補由非均質垂直速度標準偏差造成之漂移速度具彌補程度大而使得作物葉覆區內顆粒沈澱過程顯著。經由質量守恒測試之模式鑑定顯示第一階馬可夫鏈加水水平及垂直方向紊流速度之相關性之隨機步行模式為最佳。最後便利用第一階馬可夫鏈加紊流速度相關性為主之隨機步行模式描述一考慮大氣穩定狀況及紊流之傳輸與沈澱模式。選擇一相關大豆田中噴灑水滴顆粒傳輸之文獻實例以驗證本傳輸與沈澱模式。由研究文獻所得之量測資料與模式預測之顆粒濃度分佈比較結果顯示本模式可合理地預測植物葉覆上及內層之顆粒分佈。

關鍵詞：氣懸顆粒，傳輸與沈澱模式，隨機步行模式，紊流，植物葉覆。

### ABSTRACT

In order to describe a transport model to predict micrometeorological layer/surface airborne particle distributions over agricultural fields, the turbulent structure in a crop field was modeled and a new Random Walk model in terms of a Markov chain concept was presented. A new Random Walk model considers inhomogeneous turbulent flow with non-zero gradient of standard deviation of vertical velocity and skewness of turbulent velocity in the vertical direction was developed and compared to other Random Walk models. Simulation results show skewness of turbulent velocity not only compensates for the drift velocity caused by inhomogeneous of standard deviation of vertical velocity, but the magnitude of compensation is so large that it results in the significance of particle deposition process in the canopy region. Model verification via a mass conservation test shows the first-order Markov chain with turbulent velocity correlation between horizontal and vertical directions works best. A transport and deposition model which con-

siders atmospheric stability conditions and turbulence of airflow was presented using the first-order Markov chain with turbulent velocity correlation. A model case obtained from research literature regarding to the spray droplet transport in a soybean field was chosen to verify the transport and deposition model. Comparison between measured data from research literature and predicted concentration distributions from model show reasonable prediction of particle distributions above and within a plant canopy.

**Keywords:** airborne particle, transport and deposition, random walk model, turbulence, plant canopy.

## Introduction

Many particle dispersal problems of interest in agriculture, such as the dispersal of plant pathogen spores, pollen, in splash droplets and the transport of crop spray droplets in an agricultural field, are connected with heavy airborne particles that do not follow the high-frequency turbulence.

Most transport models which have been reported do not consider the effect of turbulent air flow on the transport and deposition of airborne particles above and within a plant canopy. Turbulence changes randomly with aerodynamic properties of a plant canopy and the surrounding meteorological conditions. Sometimes the upper portion of a plant canopy prevents transport into the lower part and causes poor uniformity and low deposition of particles on the agricultural fields. Air turbulence and plant canopy characteristics are major factors which influence transport mechanisms of airborne particles. Airborne particle transport and deposition under highly inhomogeneous turbulence caused by a plant canopy can be simulated by a Random Walk modeling technique because the Random Walk model sufficient flexibility to involve mass transfer of a particle dynamics, and the random effect due to turbulence on particle motion (Legg, 1983; Bughton, 1987; Picto et al., 1986; Walklate, 1986, 1987). The difficulty of developing a Random Walk model is how to describe the turbulence characteristics realistically.

Air flow above and within a plant canopy is

inherently turbulent. The most obvious property affecting airborne particle transport is the mean horizontal velocity. Turbulence properties of wind such as the Lagrangian time scale and turbulence intensity have been considered important parameters for describing turbulent flow (Raupach and Thom, 1981).

There has been a tremendous amount of work on atmospheric convection in the boundary layer. In large scale transport modeling, the presence of a plant canopy affects only the roughness length. Micrometeorological properties in a plant canopy, however, are of concern to researchers who are interested in particle above and within a plant canopy. A relatively small number of researchers have studied turbulence characteristics above and within a plant canopy (Raupach and Thom, 1981; Legg and Moniteith, 1975; Bradley and Finnigan, 1973; Thom, 1975). Some common characteristics are found: (1) turbulent air flow within and above a plant canopy are different; and (2) the turbulence characteristics within canopy are not fully understood.

In most transport modeling, representation of real turbulences is limited. This fact determines the reliability of the transport model. The Random Walk model (Hall, 1975; Wilson et al., 1981, Legg, 1983; Walklate, 1987, Picto et al., 1986), however, can handle the entire transport process by assuming a local homogeneity with the bias velocity term or by generating a non-Gaussian number which satisfies the turbulence structure.

In specific terms, the purposes of this paper are: (1) To present a transport/deposition model of airborne particles under turbulent atmospheric flow above and within a plant canopy using the Random Walk modeling technique. (2) To prove the validity of the turbulent transport model by comparing the predicted dispersion of the airborne particle with a research literature.

## Random Walk Modeling

### Micrometeorological Modeling of Turbulence

Before modeling micrometeorological above and within a plant canopy, it was necessary to determine variability of the wind velocity. The most dominant transport parameter is mean wind profile. Developing reliable wind profile requires a tremendous amount of experimental data. Mean wind velocity profile above the canopy height ( $H_c$ ) was already developed by many researchers. A logarithmic wind profile considering atmospheric stability conditions was chosen. Best curve-fitting zero-plane displacement ( $d$ ) and roughness length ( $z_0$ ) were chosen using the literature data for a typical crop field:  $z_0/H_c$  and  $d/H_c$  were 0.066 and 0.73, respectively (Raupach and Thom, 1981). Therefore, the mean wind velocity profile above and within a plant canopy can be expressed by:

$$U(z) = \begin{cases} (u_*/4) \ln((z - 0.73H_c)/Z_0 - \psi(z - 0.73H_c)/L), & z > H_c \\ (u_*/4) \ln((H_c/0.066H_c - \psi(z - 0.73H_c)/L) \cdot \exp(1.3(z/H_c - 1))), & z \leq H_c \end{cases} \quad (1)$$

where:

$$\psi = \begin{cases} 21 \ln((1 + 1/\phi_M)/2) + \ln((1 + 1/\phi_M^2)/2) - 2 \tan^{-1}(1/\phi_M) + \pi/2, & L < 0 \\ -4.7z/L, & L \geq 0 \end{cases} \quad (2)$$

$$\phi_M = \begin{cases} (1 - 15z/L)^{-1/4}, & L < 0 \\ 1 + 4.7z/H, & L \geq 0 \end{cases} \quad (3)$$

The Monin-Obukhov length ( $L$ ) in Eqn. 1 can be approximately determined once the roughness length and the stability conditions are known (Golder, 1972).

In Random Walk modeling, researchers have attempted to find the Lagrangian time scale ( $T_L$ ) in estimating the order of Lagrangian time scale from field data or Eulerian time scale ( $T_E$ ), set the range of Lagrangian time scale and then simulate a Random Walk model by changing the Lagrangian time scale with a small time step and find a Lagrangian time scale value that produces the best estimate. The Eulerian time scale can be modeled as a linear equation as follows (Hinze, 1975);

$$T_E = \begin{cases} 0.78, & z < 0.3H_c \\ 1.38, & z > 1.6H_c \\ 0.46(z/H_c - 0.3) + 0.78, & \text{else} \end{cases} \quad (4)$$

Hanna (1981) reported that the ratio of  $T_E$  and  $T_L$  is related to turbulence intensity (TI) and suggested the following equation:

$$T_L/T_E = 0.74U(z)/\sigma_w(z) = 0.74/TI(z) \quad (5)$$

Larger turbulence intensity implies existence of large scale eddies. In this study, standard deviation of wind in the  $z$ -direction was the most important parameter for vertical dispersion of airborne particles. Therefore, turbulence intensity in this study can be defined as:  $TI(z) = \sigma_w(z)/U(z)$ , where:  $\sigma_w$  = standard deviation of wind velocity in  $z$ -direction ( $w$ ). Furthermore, turbulent intensity can be expressed as a linear equation above and within a plant canopy (Legg and Raupach, 1982; Walklate, 1987):

$$TI = \begin{cases} 0.58, & z < 0.3H_c \\ 0.25, & z > 1.6H_c \\ 0.254(z/H_c - 0.3) + 0.58, & \text{else} \end{cases} \quad (6)$$

As can be seen from Eqns. (4) and (5), the estimated Lagrangian time scale then can be modeled as follows:

$$T_L = \begin{cases} 0.9414, & z < 0.3H_c \\ 3.864, & z > 1.6H_c \\ 1.284/(0.656 - 0.254z/H_c) - 1.273, & \\ \text{else} & \end{cases} \quad (7)$$

### Model Structure

A Random Walk model which was the first-order Markov chain has been successful in simulating gaseous transport. In order to simplify the model, several assumptions were made: (1) a two-dimensional wind direction (x- and z- direction) is defined and the y-component of turbulence on the transport of particles is negligible; (2) fluctuating components  $u$  and  $v$  are distributed with Gaussian distribution; and (3) turbulence in the x-direction is homogeneous.

A Markov chain for turbulent wind velocity is the Lagrangian expression of turbulent wind velocity. Taylor (1921) pointed that a Gaussian random effect in the simple Markov chain caused the drift velocity (i.e., negative mean velocity in the z-direction) in turbulent flow having non-zero  $\partial\sigma_w^2/\partial z$ . Several researchers presented new Markov chain for turbulent wind velocity when  $\sigma_w$  is not constant with height. The new Markov chain include a bias velocity term which compensates for drift velocity.

Ley (1982) determined an additional acceleration caused by the pressure gradient and added this acceleration in his Markov chain. By integrating the new equation, the following equation can be obtained (Legg and Raupach, 1982):

$$w(t + \Delta t) = \alpha w(t) + (1 - \alpha^2)^{1/2} \sigma_w \xi_n + (1 - \alpha) T_L \partial\sigma_w^2/\partial z \quad (8)$$

in which  $\alpha$  is the Lagrangian velocity correlation during Lagrangian time step ( $\Delta t$ ) and can be defined as:  $\alpha \equiv \exp(-\Delta t/T_L)$ ; and  $\xi =$  Gaussian random number.

Experimental data (Raupach, 1989) showed that within a plant canopy,  $\partial\sigma_w^2/\partial z$  term has a nearly constant positive value but skewness of turbulent velocity increases with height from the ground. If a negative skewed distribution is assumed in turbulent flow with positive gradient of  $\sigma_w^2$ , skewness of turbulent velocity becomes a smaller negative value as height decreases. Therefore, the drift velocity can be eliminated when skewness of velocity changes with height. In this modeling, experimental data obtained by Raupach (1989) on skewness and gradient of  $\sigma_w^2$  in the z-direction were used. Skewness of wind velocity in the z-direction therefore can be modeled as a linear equation (Raupach, 1989):

$$SK_w = \begin{cases} 0.1, & z \geq 1.6H_c \\ -0.78, & z < 0.3H_c \\ 0.677(z/H_c - 0.3) - 0.78, & \text{else} \end{cases} \quad (9)$$

Term  $\partial\sigma_w^2/\partial z$  was determined from Eqns. (1) and (6) as follows:

$$\partial\sigma_w^2/\partial z = \partial[(TI(z) \cdot U(z))^2]/\partial z \quad (10)$$

Detailed descriptions of the x-direction Markov chain slows simulation speed. In this modeling, the horizontal turbulent wind velocity was modeled by a simple Markov chain. The proposed Markov chain in the x- and z-directions are as follows:

$$u_{i+1} = \alpha u_i + (1 - \alpha^2)^{1/2} \sigma_u \xi(0, 1, 0) \quad (11)$$

$$w_{i+1} = \alpha w_i + (1 - \alpha^2)^{1/2} \sigma_w \xi(0, 1, SK_w) \quad (12)$$

Eqns. (11) and (12) are referred to as Model-I. Parameters of the two random numbers,  $\zeta$  and  $\xi$  are mean, standard deviation, and skewness, respectively.

In model-I, skewness of the vertical wind component was modeled to improve performance of the first order Markov chain in inhomogeneous turbulence, where velocity fluctuation shows non-zero skewness. Inclusion of skewness reduced simulation speed. As a compromise for speed and accuracy, skewness was considered only for the fluctuating wind in vertical direction, which contributes to the vertical dispersion of airborne particles.

One Random Walk model (Legg and Raupach, 1982) was selected to compare performance of Model-I to an existing model. Legg and Raupach's model is referred to as Model-II. The Model-II is described as follows:

$$u_{i+1} = \alpha u_i + (1 - \alpha^2)^{1/2} \sigma_u \xi(0, 0, 0) \quad (13)$$

$$w_{i+1} = \alpha w_i + (1 - \alpha^2)^{1/2} \sigma_w \xi(0, 0, 0) + (1 - \alpha) T_L \partial \sigma_w^2 / \partial z \quad (14)$$

In Model-I and Model-II,  $\sigma_w$  could be determined from the mean wind velocity by using the definition of turbulence intensity (i.e.,  $\sigma_w(z) = TI(z) \cdot U(z)$ ); whereas  $\sigma_u$  could be determined from the ratio of  $\sigma_w/\sigma_u$  as follows (Walklate, 1987):

$$\sigma_w/\sigma_u = \begin{cases} 0.72, & z > 1.6H_c \\ 1.42, & z < 0.3H_c \\ 0.538(0.3 - z/H_c) + 1.42, & \text{else} \end{cases} \quad (15)$$

Therefore, a new Random Walk model was proposed which considers skewness of turbulent velocity in the z-direction and used for developing a transport and deposition model.

## Transport and Deposition Modeling

### Transport Modeling

Mass transport of an airborne particle above agricultural fields has been developed by Goering et al. (1972) who used a nonlinear differential equation to describe the particle transport dynamics:

$$dD_p/dt = -2(M_v/M_m)(D_v/D_p)(\rho_d/\rho_l)(\Delta p/p_a) \cdot (2 + 0.6N_{sc}^{1/2} N_{Re}^{1/2}) \quad (16)$$

where:  $D_p$  = particle diameter;  $M_v$  = molecular weight of water vapor;  $M_m$  = mean molecular weight of gas mixture in transfer path;  $D_v = 0.528 \cdot 10^{-5} T_k$  ( $T_k$  = temperature in  $^{\circ}K$ ), diffusivity of water vapor in air;  $\rho_a$  = air density;  $\rho_l$  = liquid density in the particle;  $\Delta P$  = vapor pressure difference;  $P_a$  = air partial pressure;  $N_{sc}$  = Schmidt number ( $\equiv D_v/\nu_a$ ); and  $N_{Re}$  = Reynold's number ( $\equiv V_r D_p/\nu_a$ );  $V_r$  = velocity of particle relative to air;  $\nu_a$  = kinetic viscosity of air.

Velocity of an airborne particle ( $V_p$ ) was modeled as a non-linear first-order differential Equation (Goering, et al., 1972):

$$mdV_p/dt = F - V_e dm/dt \quad (17)$$

$$F = g(\rho_p - \rho_a) \pi D^3 / 6 + 1/2 (C_d \rho_p A_p V_r^2) \quad (18)$$

Where:  $V_e$  = velocity of ejected mass relative to the particle ( $V_e = -V_r$ );  $A_p$  = projected area of a particle ( $1/4 \pi D_p^2$ ). The drag force (F) is related to the relative velocity of a particle with respect to air velocity ( $V_r$ ). Thus, two differential equations expressing x- and z-directional velocity must be solved simultaneously.

Drag coefficient ( $C_d$ ) of a particle was calculated by using the standard drag coefficient curve for a sphere (Cliff et al., 1978). Various models for drag coefficient of a single sphere have been published (Yen and Tu, 1966; Ishii and Zuber, 1979; Cliff et al., 1979).

Differential equations for dynamics of a

particle and for mass transfer were solved using the fourth-order Runge-Kutter integration method.

### Deposition Modeling

Airborne particles are heavier than air so that particles iminging on a target may bounce-off a waxy surface, disintegrate into smaller particles, be deposited and remain on the surface or be resuspended from th surface (Hinds, 1982). In this study, the bounce-off, disintgrtion and reentrainment of particles were neglected. The three deposition mechanisms Considered were eddy diffusion, inertial impaction and settling. For convenience, the three mechanisms will be termed as impaction.

**Determination of impaction coefficient:** The plant canopy was assumed to be an assembly of cylindrical targets (petioles and stems) and long ribbon type target (leaves). The geometrical shape of a leaf is similar to a disc. Impaction efficiency for a cylindrical target ( $\eta_{cyl}$ ) and a long ribbon ( $\eta_{nb}$ ) were modeled as follows respectively (May and Clifford, 1967):

$$\log(\eta_{cyl}) = \begin{cases} 0.6 + 0.988\log(St) + 0.413\log^2(St) & \text{for } St \leq 0.6 \\ 0.546 + 0.562\log(St) - 0.242\log^2(St) & \text{for } ST \geq 0.6 \end{cases} \quad (19)$$

$$\log(\eta_{nb}) = \begin{cases} 0.692 + 1.389\log(St) + 0.707\log(St) & \text{for } ST \leq 0.6 \\ 0.544 + 0.567\log(St) - 0.194\log^2(St) & \text{for } St \geq 0.6 \end{cases} \quad (20)$$

where:  $St = \rho_p U_p D_p^2 / (18 \nu_a L_e)$  (Stokes number): in which,  $U_p$  = mean particle velocity; and  $L_e$  = characteristic length of leaf and petiole (May and Clifford, 1967).

**Determination of deposition probability:** The probability of particle deposition ( $P_d$ ) can

be calculated for every simulation step when a particle is within a plant canopy or for certain vertical movement. In order to save computation time, the second case was chosen. The vertical displacement ( $X_v$ ) or horizontal distance ( $X_h$ ) demanding a new deposition probability was 0.1 m except in the top of the canopy where the distance was 0.05 m. Once either  $X_h$  or  $X_v$  was greater than 0.1 m, deposition probability was recalculated and the displacement in the other direction was determined by mean horizontal or vertical particle velocity (Fig. 1).

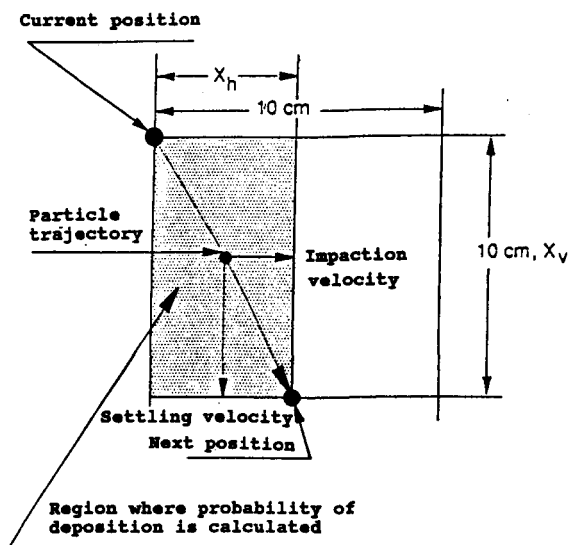


Fig. 1. Schematic representation of particle impaction

Particle deposition probability is determined by multiplication of impaction efficiencies of foliage ( $\eta_f$ ) and of petiole ( $\eta_p$ ), and therefore a probability of target existence in a given vertical movement can be expressed as:

$$P_d = P_f \eta_f + P_p \eta_p \quad (21)$$

where:  $P_f$  and  $P_p$  are the fraction of foliage density (foliage area/m<sup>3</sup>) and fraction of petiole density (cylindrical target area/m<sup>3</sup>) respectively. Impaction by horizontal motion of a particle was modeled with Eqns (19) and (20). Impaction by vertical motion (settling) was assumed to be unity.

The probability of travel without deposition within the given space is:

$$\begin{aligned}
 1 - P_d &= (1 - P_{d,v})[1 - P_{d,h}(X_h/X_v)] \\
 &= 1 - P_{d,v} - P_{d,h}X_h/X_v + P_{d,v}P_{d,h}X_h/X_v
 \end{aligned}
 \tag{22}$$

Thus, particle deposition probability can be expressed as (Fig. 1):

$$P_d = P_{d,v} + P_{d,h}X_h/X_v - P_{d,v}P_{d,h}X_h/X_v \tag{23}$$

where:

$$P_{d,h} = \eta_f P_{f,h} + \eta_p P_{p,h} \tag{24-1}$$

$$P_{d,v} = P_{f,v} + P_{p,v} \tag{24-2}$$

**A plant canopy modeling:** Determination of deposition probability requires fraction of foliage and petiole densities as a function of height. The fraction of the foliage and petiole densities must be calculated in the horizontal and vertical directions at every height. Fig. 2 shows the plant structure definition (Hommertzheim, 1979) for a plant canopy. The fractions of the foliage and petiole densities in the horizontal and vertical directions were calculated and are shown in Fig. 3 (Hommertzheim, 1979).

When an airborne particle entered the plant canopy, the deposition probability was calculated at every given vertical movement (0.1 m except at the top of a plant canopy). An uniform random number between 0 and 1 was also generated. If the random number is smaller or equal to the  $P_d$ , the particle was assumed to be deposited on the plant canopy and turbulent transport and deposition simulation for the particle was terminated. If the particle traveled the given vertical distance without deposition, then the simulation continued until the particle deposited or reached the ground.

**Structure of transport and deposition**

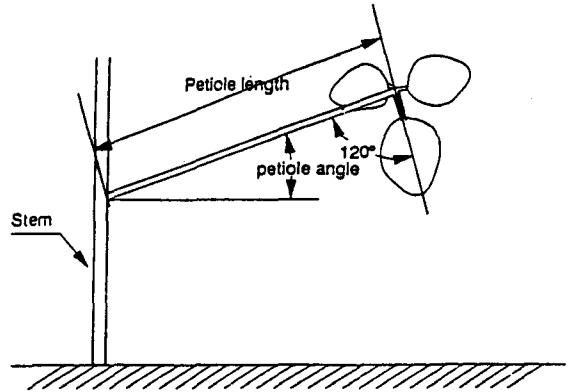
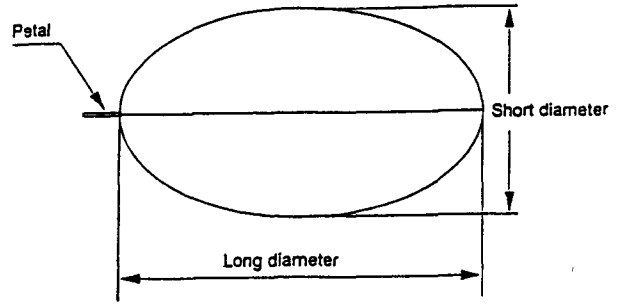


Fig. 2. Definition of a plant structure (soybean).

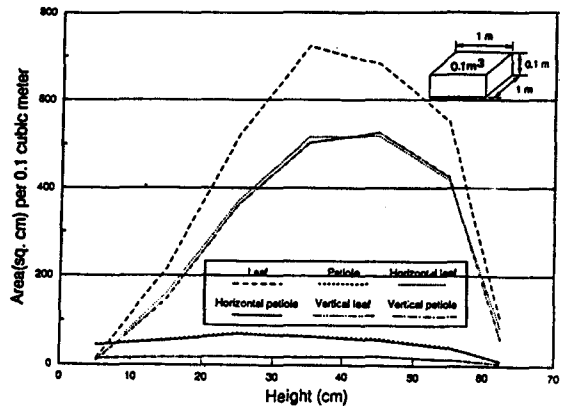


Fig. 3. Fractions of foliage and petiole density of plant canopy in the horizontal and vertical direction.

**model:** The transport and deposition model was programmed in Quick C Version 2. (Microsoft). The overall structure of the program can be stated as follows: First, the executable program

reads the input file and calculates physical and meteorological properties required in the model. It simulates the trajectory of air-borne particles and determines the location of an airborne particle at different heights under mean horizontal wind. The next step is to generate an angle of airborne particle sources using a Gaussian random number generator and simulate one trajectory at a time. Initially, a particle has high velocity and laminar transport is used. When particle velocity is 20 times less than  $\sigma_w$ , turbulent effect is considered. If the particle is within the plant canopy, the deposition process is used. Deposition or passing over targets is decided very 10 cm in either the vertical or horizontal displacement.

### Model Verification

Verification of the transport and deposition for airborne particles can be divided into two phases. The first phase is verification of Random Walk model performance: To prove the model satisfies mass conservation at every height. The second phase is verification of transport and deposition model: To compare predicted results to measured data obtained from research literature.

### Random Walk Model Simulation

**1. Determination of simulation step:** Accuracy of a Random Walk model is affected by proper determination of the Markov chain time step, which is related to Lagrangian integral time step. The Lagrangian integral time scale ( $\Delta t$ ) is interpreted as the time during which Lagrangian particle velocities are significantly correlated (Fig. 4). Distances where Lagrangian particle velocities are correlated are represented by the Lagrangian integral length scale: x-direction =  $(U + u)\Delta t$ ; and z-direction =  $\sigma_w \Delta t$ . When turbulent velocities at a point are generated by a Random walk model, the turbulent velocities are valid inside a region surrounded by the Lagrangian integral length scale (Fig. 4).

Markov chain time step ( $\Delta t$ ) is usually

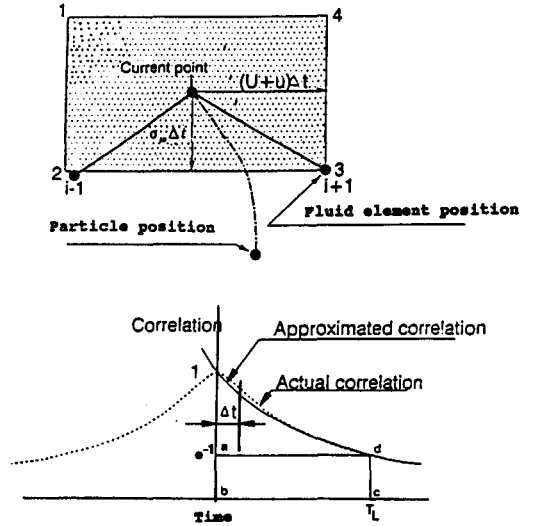


Fig. 4. Schematic of a particle trajectory and determination of proper Markov chain time step.

determined between  $0.125T_L$  and  $0.2T_L$  (Legg, 1983) (Fig.4). Markov chain time step drastically affects the speed of simulation. If  $\Delta t$  is too large, accuracy of the Markov chain will be decreased.

**2. Initial and boundary conditions:** Position of a particle can be expressed as:  $x_i = x_{i-1} + u_i \Delta t$  and  $z_i = z_{i-1} + w_i \Delta t$ ; initial conditions are:  $x = 0$ , at  $t = 0$  and  $z = H_c - 0.1$  at  $t = 0$ ; and turbulent velocities in both directions were assumed to be initial particle velocities in both directions; i.e.,  $u_p(t = 0) = U_{p,init}$ ; and  $w_p(t = 0) = W_{p,init}$ . Three kinds of boundary conditions were used: (1) a totally reflecting boundary layer: set at  $z = 5$  m to restrict the simulation region close to the ground. (2) a totally absorbing boundary layer: set at  $z = 0$  (ground). (3) a partially absorbing boundary layer: between the ground and the plant canopy height.

**3. Random number generator:** Two random number generators which utilize three linear congruential generators with a shuffle routine were used (Dagpunar, 1988). A total of six linear congruential random number generators were employed for the random number generation. The two random number ( $R_1$  and  $R_2$ ) from the two



generators we re used to make a single Gaussian random number which has zero mean with stand- are deviation of unity using the Box-Muller method (Dagpunar, 1988):

$$X_1 = (-2\ln(R_1))^{1/2} \cos(2\pi R_2) \quad (25)$$

In the Random Walk model-I, vertical fluctuation was assumed to have a skewed Gaussian distribution. The transformation equation of a Gaussian random number ( $X_1$ ) to a skewed random number ( $Z$ ) was (Dagpunar, 1988):

$$Z = 1/\sigma_X [(X_1 + 3.05)^P X - M_X] \quad (26)$$

Transform parameters,  $P_X$ ,  $M_X$ ,  $\sigma_X$  were modeled as a function of skewness of the transformed Gaussian random number as a third-order polynomial equation (Knuth, 1981).

Two sets of random numbers with correlation between them are necessary in the simulation in order the simulate correlation between horizontal and vertical wind components. To transform independent Gaussian random numbers ( $X$ ) into two dependent Gaussian randoms ( $Y$ ), the following transformation was used. The matrix  $C$  can be obtained by the Cholesky decomposition of the covariance matrix of  $X$  (Dagpunar, 1988);  $Y = C X + 0$ ; where, the matrix  $C$  is:

$$C = \begin{pmatrix} \sigma_u^2 & 0 \\ \sigma_{uw}/\sigma_u & (\sigma_w^2 - \sigma_{uw}^2/\sigma_u^2)^{1/2} \end{pmatrix} \quad (27)$$

**4. Mass conservation test:** In order to determine the best performing model, two Random Walk models: Model-I with correlation between two turbulent velocities, and Model-II were utilized. Atmospheric stability was set to be neutral. Turbulence structure above and within a plant canopy, as describing in the modeling section was used. In order to check mass conservation in the Random Walk model, 50 point sources were assumed from 0.05 to 4.95 m above the ground at

0.1 m interval and the concentration profile of particles at various downwind distances were investigated. The concentration profile indicates not only mass conservation in the model but consistency of model behavior with respect to height above the ground.

Three thousand paths of particles were simulated for each point source. Therefore, the total number of simulations was 150,000. At the source point, turbulent velocity was assumed to be zero. The position of each particle was termied at 1 m intervals downwind to a distance of 5 m. To reduce simulation time, totally reflecting boundary layers were set at ground level and at 5 m above the ground.

Fig. 5 shows the concentration profile

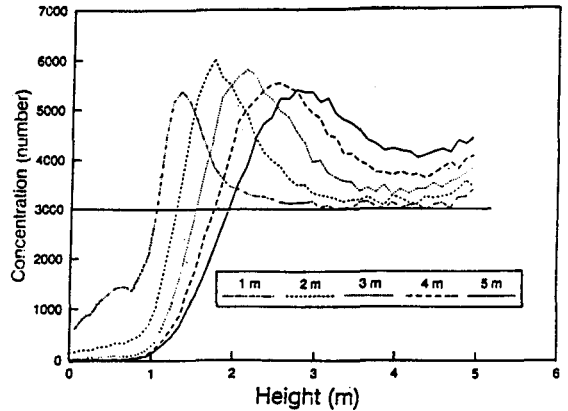


Fig. 5. Particle concentration profiles predicted by the Model-II at various downwind distances.

predicted by Model-II. The figure shows a large negative drift velocity in the concentration profile. Discrepancies near the canopy region is very large indicating that this model and the developed turbulence structure appear to be improper for a plant canopy. Legg and Raupach (1982) tested the model against wind tunnel data and indicated that the Model-II maintains a constant concentration profile within height. The reason for the severe negative drift velocity seems

to be due to the existence of a deterministic bias velocity. The existence of a positive gradient of  $\sigma_w^2$  in the z-direction will continue to pull particles in the upwind direction.

Fig. 6 shows the concentration profile predicted by Model-I. The figure shows considerable discrepancies within the plant canopy but small discrepancies are observed as the downwind distance increases. The Model-I shows about 15% error in predicting particle concentrations. The good performance of the Model-I is due to short simulation distances and inclusion of the correlation between the two turbulent velocities. One difference between Figs. 5 and 6 is that the Model-II shows many peaks while Model-I shows only one peak in the concentration profile. Generally, the Model-I with correlation between turbulent velocities worked best. For model development purposes, the Model-I was chosen.

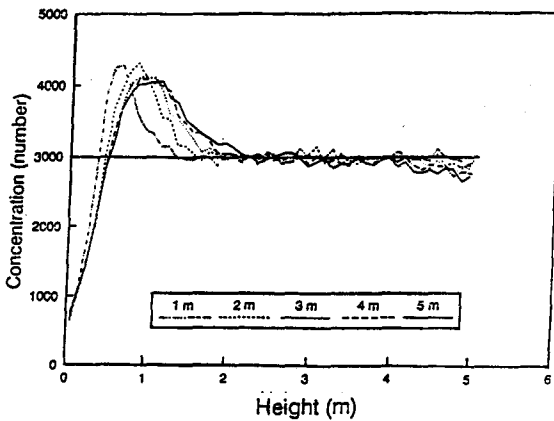


Fig. 6. Particle concentration profiles predicted by the Model-I at various downwind distances.

### Transport and Deposition Model Simulation

**1. Model case description:** A model case will be studied in some details to give insight into the behavior of transport and deposition of particles over a crop field. The model case is chosen from the paper entitled: "Transport of Spray Droplets

from Flat-Fan Nozzles" by Rhee et al. (1990).

In order to simulate transport and deposition of spray droplets, the true droplet spectrum, droplet velocities and drop size at the initial condition are required. In actual field spraying, there is generally horizontal wind. The horizontal wind will encounter the spray jet and distort its shape. A study by Rhee et al. (1990) shows that the shape and size of a horizontal section of the spray jet can be assumed to be the same as those in no-wind condition while the section was moved in the horizontal direction by wind (Fig. 7). Entrained air velocity will be

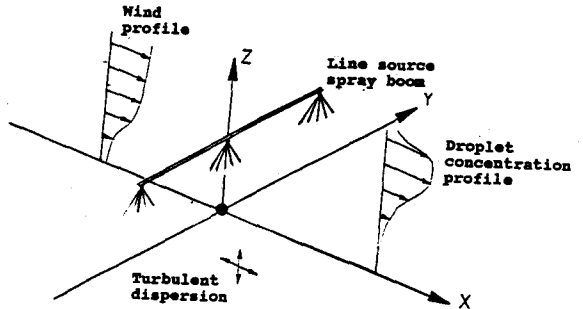


Fig. 7. Coordinate system in transport and deposition modeling of spray droplets above and within a soybean canopy according to the research literature (Rhee et al., 1990).

different depending on the position inside the spray jet. The entrained air velocity inside the spray jet can be specified using two geometrical parameters such as angles  $A_f$  ( $0^\circ-40^\circ$ ) and  $A_d$  ( $0^\circ-13^\circ$ ) (Fig. 8).

By assuming the same entrained air velocity profile in the direction of angle  $A_d$ , the entrainment air velocity at a specific position ( $V_{e,s}$ ) can be expressed as follows (Rhee et al. 1990):

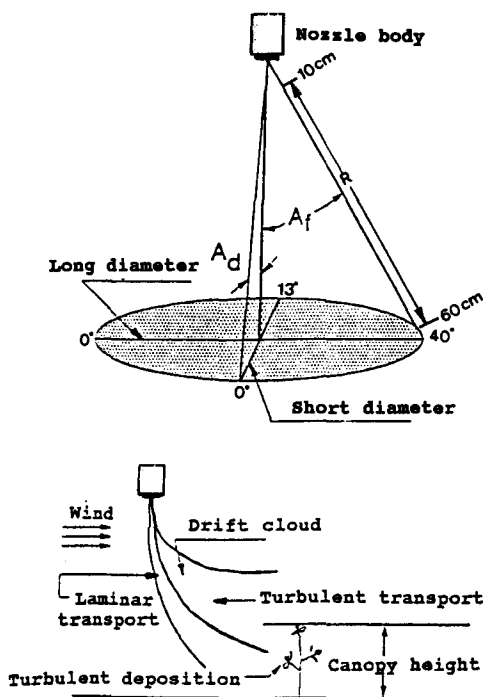


Fig. 8. Entrained air flow and droplet separation in a spray jet under a field condition. Top: Geometric configuration of angles  $A_f$  and  $A_d$ . Bottom: Schematic presentation of droplet separation in the side-view section.

$$V_{e,s} = V_{en} (-0.00022A_f^2 + 0.99) (-0.005858A_d^2 + 0.99) \quad (28-1)$$

where velocity of entrained airflow in spray jet ( $V_{en}$ ) can be expressed as

$$V_{en} = [(-1.0239P_n - 0.5204)\log R + (1.8337P_n - 2.1589)] (-0.000228A_f^2 + 0.99) \quad (28-2)$$

where:  $P_n$  = operating pressure at a nozzle tip (bar), and  $R$  = radial distance from a nozzle tip (10 – 60 cm).

Without experimental verification, it was assumed that the dispersion rate is linearly proportional to the depth of plant canopy. Entrained air velocity within a plant canopy was

expressed as follows (Rhee et al. 1990):

$$V_{e,s}|_{z < H_c} = (z/H_c)V_{en} \quad (29)$$

Spray volume in the  $A_d$ -direction can be approximately by a Gaussian distribution function (El-Awady, 1976) (i.e., the angle,  $A_d$ , for each droplet was generated by a Gaussian random number generator).

In this simulation, only airborne droplet spectrums were verified with experimental data obtained from research literature. The reason for this is difficulty in obtaining accurate measurement. Many research literatures (Rhee et al., 1990; Raupach et al., 1986) show that it is possible to measure deposits on plant leaves. Even detailed information such as droplet number and size are measurable. The deposited droplet size, however, is not the same as that of impacted droplets because of splash, split and bounce-off of droplets from a targets is strongly related with impaction speed, droplet size and target surface characteristics (Hinds, 1982).

The measured airborne spectrum had significant limitations in interpretation of the simulation results. Therefore, model verification is inevitably a partial verification.

**2. Input conditions:** The model was programmed to obtain size and vertical position at specified distances. Points selected were 2, 3, and 5 m from the sprayer in the downwind direction. The simulation program requires three categories of input data: (1) initial droplet size spectrum and droplet velocity, (2) meteorological data, (3) operating conditions such as nozzle height, pressure and orientation. Three different meteorological data (Rhee et al., 1990) were used as an input for simulation: (I): dry-hulb temperature ( $T_{db}$ ) = 22°C, wet-bulb temperature ( $T_{wb}$ ) = 13°C, friction velocity ( $u_*$ ) = 0.35 m/s, stability = neutral; (II):  $T_{db}$  = 19°C,  $T_{wb}$  = 14°C,  $u_*$  = 0.4 m/s, stability = slightly stable; (III):  $T_{db}$  = 23°C,  $T_{wb}$  = 15°C,  $u_*$  = 0.2 m/s, stability = slightly unstable.

The other information such as  $\sigma_u$  and  $\sigma_w$

were estimated using the proposed equations in the model development. Operating pressure at the spray boom was 2 bar and nozzle height was 1 m from the ground (Rhee et al., 1990). The spray boom was stationary. Literature data of the true droplet size spectrum and initial droplet velocity were inputs of the simulation program. The initial point was 0.1 m below the sprayer nozzle. Two different droplet sizes of 50 and 150  $\mu\text{m}$  in diameter were selected for model verification.

**3. Comparison with research literature:** The transport and deposition model utilized the Random Walk Model-I with the turbulent velocity correlation, which performed best for mass conservation. Skewness turbulence for the model was based on the suggested model. Fig. 9 shows the concentration profile of 50  $\mu\text{m}$

figure shows that the model over-predicted the droplet concentration 1 m above the ground. This difference was caused by the fact that the transport and deposition model simulates the droplet even after the droplet is totally evaporated.

Figs. 10 and 11 show predicted profiles of

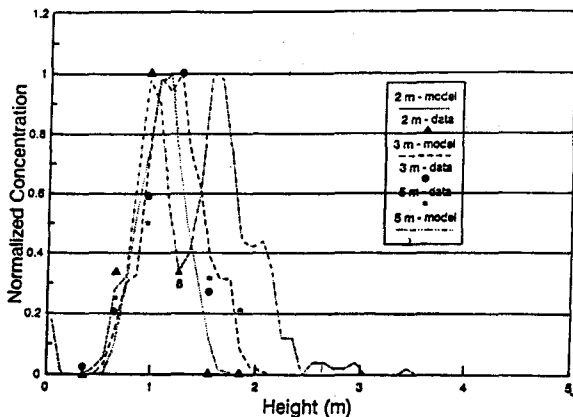


Fig. 9. Normalized concentration profile of 50 micron droplets under a neutral condition at various downwind distances.

droplet at 2, 3, and 5 m downwind distances as predicted under Simulation-I conditions. The concentration of droplets were normalized by their maximum values (1000 particle number). The figure shows that dispersion of droplets increases as downwind distance increases. Dispersion in the negative z-direction appears to decrease due to the deposition of droplet. The

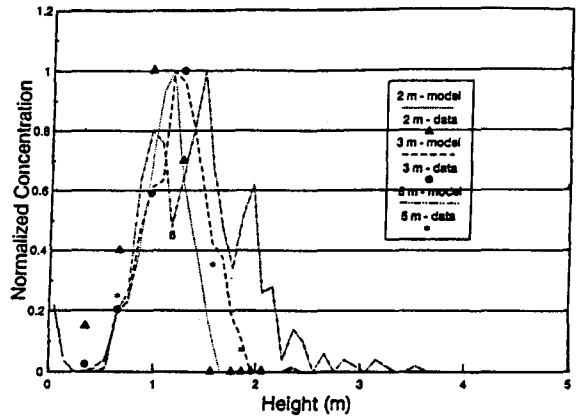


Fig. 10. Normalized concentration profile of 50 micron droplets under a slightly unstable condition at various downwind distances.

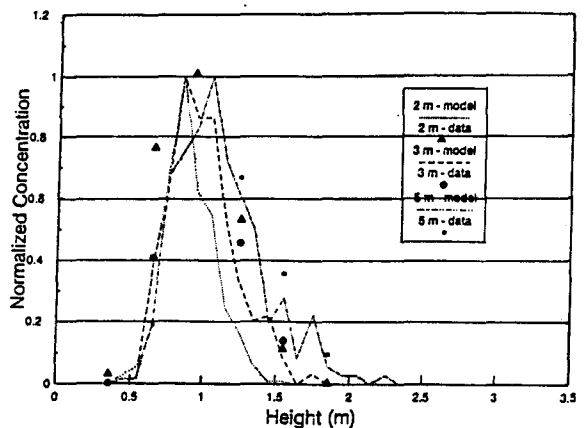


Fig. 11. Normalized concentration profile of 50 micron droplets under a slightly stable condition at various downwind distances.

droplet concentration under the conditions of Simulation-II and Simulation-III. As can be seen from Figs. 10 and 11 that the normalized concentration predicted by the model are very close to the measured data of research literature below the center of spray droplet plume. Above the center of the plume, the model over-estimated droplet concentration. Figs. 9, 10, and 11 show that droplet concentration profiles have multiple peaks as the downwind distance increases. The concentration profile appears to be separated at a point  $\beta$ . This phenomenon is due to the difference of totally evaporated and evaporating droplets in dispersion.

Fig. 11 shows the minimum separation in concentration profile because the mean velocity under the condition of Simulation-II had highest values among the three conditions. The droplets under the conditions of small turbulence intensities reached a specific position in a short time. Measured droplet concentrations indicate how much droplet dispersion is affected by the simulation conditions. Close observation of Figs. 9, 10, and 11 reveals that droplet concentration under conditions of Simulation-II (slightly stable), shows less dispersion compared to the droplet concentration under of Simulation-III (slightly unstable). The model, however, does not show a clear difference in the concentration profile under the three simulation conditions.

Fig. 12 shows normalized concentration profiles for 150  $\mu\text{m}$  droplets under the conditions of Simulation-I (neutral). Fifteen hundred paths of droplets were simulated for the 150  $\mu\text{m}$  droplets. The figure does not show separation of the concentration profile which was shown for 50  $\mu\text{m}$  droplet. The model does not always over-estimate the concentration of droplets. The figure also shows an elevation of the maximum concentration height increases with increasing downwind distance. This is due to depletion of droplets within the plant canopy by the deposition process.

Figs. 13 and 14 show droplet concentration profiles under conditions of Simulation-II and

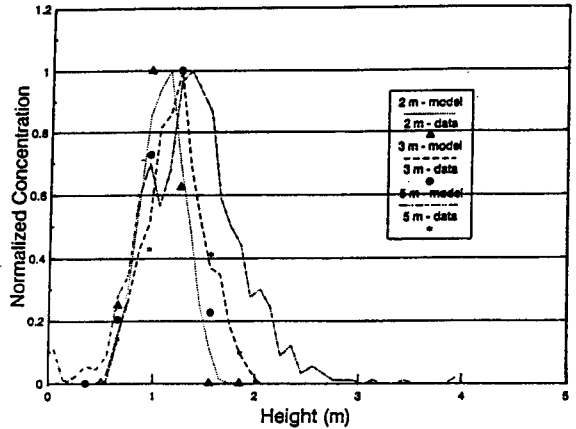


Fig. 12. Normalized concentration profile of 150 micron droplets under a neutral condition at various downwind distances.

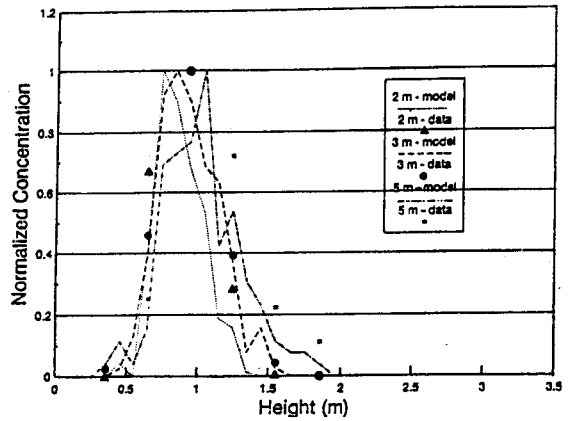


Fig. 13. Normalized concentration profile of 150 micron droplets under a slightly unstable condition at various downwind distances.

Simulation-III, respectively. Generally, the model slightly underestimates concentration of droplets. Under the slightly stable condition, the rate of elevation of the maximum concentration height is slower than that under neutral condition, while the rate of elevation under the slightly unstable condition is higher than that under the neutral condition.

### Summary and Conclusions

The following results can be drawn from this research.

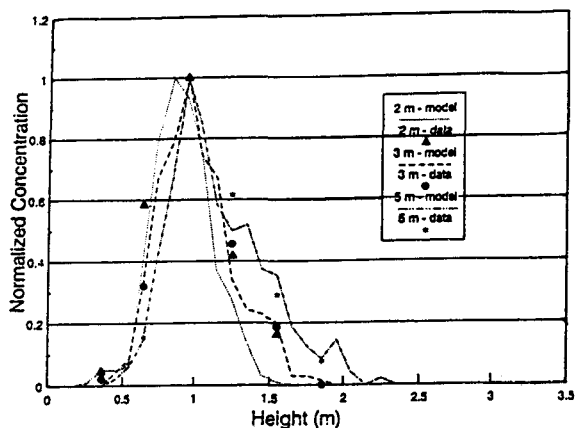


Fig. 14. Normalized concentration profile of micron droplets under a slightly stable condition at various downwind distances.

1. A new Random Walk model for inhomogeneous turbulent flow with non-zero gradient of  $\sigma_w$ , was developed and compared to other Random Walk model. Models included the simple Markov chain with turbulent velocity correlation and a Random Walk model with the bias velocity term. Model verification via a mass conservation test shows that the simple Markov chain with turbulent velocity correlation works best for the simulation of airborne particle out to 5 m in the x-direction.

2. A transport and deposition model which considers atmospheric stability conditions and turbulence of airflow was presented using the simple Markov chain with turbulent velocity correlations. A model case regarding to the spray droplet transport in a soybean field was chosen to verify the transport and deposition model. Comparison between measured data obtained from research literature and predicted concentration profiles show reasonable prediction of particle transport above and within a plant canopy.

3. Droplet deposition was not verified but the model appears to overpredict deposition in the upper part of a plant canopy. The overprediction is thought to be due to simplifying the canopy as a two dimensional structure and

neglecting impaction efficiency changes with approaching angle of the droplet.

4. The proposed model considers skewness of turbulent velocity in the z-direction. Simulation results show that skewness of turbulent velocity not only compensates for the drift velocity caused by inhomogeneous of  $\sigma_w$  in the z-direction, but the magnitude of compensation is so large that it results in depletion of particles in the canopy region. This study shows a possibility of reducing the negative drift velocity caused by skewness.

5. Skewness of vertical velocity dominantly affected the concentration profile. Negative skewness caused particles to move up. Negative stress ( $\sigma_{ww}^2$ ) enhances particle dispersion in the positive z-direction while suppressing dispersion in the negative z-direction. The Lagrangian time scale also affects the particle concentration profile.

### Acknowledgements

The author wishes to acknowledge the financial support of the National Science Council of R.O.C. under Grant NSC-82-0409-B-002-344.

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收稿日期：民國82年3月26日

修正日期：民國82年4月20日

接受日期：民國82年5月6日