

## 60. TOWARDS IMPROVING PESTICIDE DISPERSION MODELS: AN EVALUATION OF SPRAY CLOUD THERMODYNAMICS

S.L. Edburg<sup>1,\*</sup>, B.K. Lamb<sup>1</sup>, and H.W. Thistle<sup>2</sup>.

<sup>1</sup>Laboratory for Atmospheric Research, Department of Civil and Environmental Engineering, Washington State University, Pullman, WA, USA.

<sup>2</sup>USDA Forest Service, Morgantown, WV, USA.

### Abstract

Spray drift models are commonly used to determine buffer distances between target areas (e.g., crops, forests) and non-target areas (e.g., streams, neighboring crops, urban areas). Most current modeling of spray drift uses a single droplet approach that treat the atmosphere around the droplet as if it were not influenced by other droplets. This lack of a ‘neighborhood’ or ‘cloud’ effect leads to the over estimation of evaporation as the elevated humidity caused by the other droplets in the droplet cloud is not considered. Here, we evaluate spray cloud thermodynamics in an effort to improve spray drift models. We compare pesticide drift models to dense gas models over a range of ambient meteorological conditions for simple spray configurations (i.e., one nozzle with zero crosswind). Models compared well for high relative humidity but diverged for low relative humidity. We attribute the divergence to an over prediction of droplet evaporative loss in spray drift models.

### 1. Introduction

Pesticides and herbicides are commonly used for plant control (Solomon et al. 2009; Schroeder and Sturges 1980) and pest management (Fettig et al. 2008). These compounds are delivered via both air- (Ramaprasad et al. 2004) and ground-based (de Jong et al. 2000) sprayers. Pesticides and herbicides can have negative consequences for non-target areas and thus humans, terrestrial ecosystems, and aquatic ecosystems. In terrestrial ecosystems, herbicides are used for plant control, however, non-target drift can cause significant damage to nearby vegetation (Boutin and Jobin 1998). Similarly, non-target drift can negatively impact streams and thus aquatic ecosystems (Davidson and Knapp 2007).

The ideal spray application involves delivering an effective amount of spray agent (e.g., pesticide) to the target area and minimizing the amount of spray agent on non-target areas (spray drift). Buffer zones (areas where no spray is applied) are commonly used to prevent deposition to non-target areas. These zones vary in size from cm (Fettig et al. 2008) to km (Ward et al. 2006) depending on the type of agent sprayed, sensitivity of non-target area, nozzle type, spray pressure and rate, vehicle speed, and meteorology (Felsot et al. 2011; Thistle 2000). Correctly setting buffer distances can reduce spray drift onto sensitive non-target areas and thus reduce negative impacts of pesticide use.

Spray drift models are used to determine buffer distances between target areas (e.g., crops, forests) and non-target areas (e.g., streams, neighboring crops, urban areas) (Teske et al. 2011a). Most current modeling

---

\*Corresponding Author Address:  
[sedburg@wsu.edu](mailto:sedburg@wsu.edu); PO Box 2910, Pullman,  
WA, 99164-2910

of spray drift uses a single droplet approach that treat the atmosphere around the droplet as if it were not influenced by other droplets (Teske et al. 2009). However, droplets exist in clouds when sprayed into the atmosphere. We hypothesize that the lack of a ‘cloud’ effect leads to errors in evaporation because the elevated humidity caused by the other droplets in the droplet cloud is not considered. Further, the effects of expansional cooling and evaporative cooling are not included in the current applied models. These effects not only directly influence evaporation but also change the temperature of the aggregate cloud and may cause slumping.

Dense Gas models, such as the SLAB model (Ermak 1990), have existed for many years and are used to model such phenomena as material releases due to the collapse of a tank storing a volatile liquid, the crash of a tanker truck, and jet release from valve ruptures (e.g., Hanna et al. 2008). These models were originally developed to have low computational requirements. As such, most dense gas models are one dimensional (1-D) models that capture downstream dispersion of a denser than air cloud. Dense Gas models handle the cloud thermodynamics in some form. For example, SLAB captures changes in cloud temperature and turbulent mixing due to liquid droplet formation and evaporation. Although relatively simple, these models may better represent evaporative loss as compared to current spray drift models.

The objective of this study is to evaluate spray cloud thermodynamics in an effort to improve spray drift models. To do this, we compare droplet evaporation used in a common spray drift model (AgDISP, Teske et al. 2002) with the SLAB dense gas model (Ermak 1990). Downstream mass fraction is presented for a range of relative humidity (RH) to determine the difference in evaporative loss between each model.

## 2. Methods

### 2.1. Evaporation in current applied spray drift models

Current applied pesticide drift models (e.g., AgDISP, Teske et al. 2002) use a single droplet trajectory modeling approach. Droplet size distributions are handled with discrete size bins for several droplet size classes. Droplet trajectory is calculated by solving Lagrangian equations for the mean and fluctuating droplet motion (Teske et al. 2002). In these formulations, droplet size directly alters droplet motion and interaction with turbulence through the droplet relaxation time and gravity terms in the Lagrangian equation (Eqn. 2 and 3 in Teske et al. 2002).

Droplet evaporation reduces the droplet size as a function of time since release and thus alters droplet trajectory and dispersion. In AgDISP, a D-squared law (Trayford and Welch 1977) is used to calculate evaporative loss. In this approach, the droplet diameter at a future time step is

$$D_{t+1} = D_t \left[ 1 - \frac{\Delta t}{\tau_e} \right]^{1/2}, \quad (1)$$

where  $D_t$  is the droplet diameter at the previous time step,  $\Delta t$  is the time step size, and  $\tau_e$  is the evaporative time scale

$$\tau_e = \frac{2D_t^2}{\lambda \Delta \Theta Sh}. \quad (2)$$

In this formulation, the droplet time scale is related to an evaporative constant,  $\lambda$ , the wet bulb temperature depression,  $\Delta \Theta$ , and the Sherwood number,  $Sh$ , that is a function of the Reynolds number. Recent evidence has shown that this may overpredict evaporative

loss because of the lack of a cloud effect (Teske et al. 2011b). That is, the droplets behave as if they see the ambient atmosphere and not the conditions within the cloud of droplets. A different approach used in dense gas dispersion models is described in the following section.

## 2.2. Evaporation in dense gas models

Dense gas dispersion models were developed for regulatory agencies such as the EPA to predict dispersion of dense gases from accidental releases. These models have been evaluated for a variety of source types and materials (e.g., liquid natural gas, chlorine, ammonia, and aerosols; Hanna et al. 1993, 2008; Touma et al. 1995). We used the SLAB model (Ermak 1990) in this study. SLAB, similar to other dense gas models, is a 1-D model that calculates downstream droplet and vapor concentration as a function of time for various source types (e.g., area source, continuous, vertical jet, horizontal jet) by solving plume averaged conservation equations of mass, momentum, energy, and species. SLAB does not include gravitational settling or deposition of species (i.e., it is assumed that the droplet size distribution is very fine).

Droplet evaporation is explicitly treated within SLAB by assuming a local thermodynamic equilibrium between the vapor and liquid phases. First, mass conservation equations for the released material (e.g., pesticide), dry air, total water, and liquid/vapor fractions of water and released material are solved. Second, the energy conservation equation is solved. Third, the equation of state is solved for the liquid/vapor mixture. Finally, local equilibrium between phases is applied to determine the fraction in liquid and vapor phase. The local equilibrium condition requires that the vapor phase partial pressure

be less than the saturation pressure or the partial pressure of the total mass fraction in the vapor phase. Thus the droplet phase concentration is a function of the temperature and the mass fraction of emission in the cloud. Additional details and equations can be found in the SLAB users guide (Ermak 1990).

## 2.3 Numerical Experiments

We conducted model runs simulating a point release of a water-based spray for fine droplets using the SLAB model and a droplet trajectory model that uses the D-squared law for evaporation (from now on called the  $D^2$  model). In order to compare each model, we did not include gravitational settling of droplets or deposition in the  $D^2$  model. Material was released at 3 m above the ground in a steady 5 m/s wind with a range of relative humidities. For each run we examined downstream mass fraction as a function of RH.

## 3. Results and Discussion

### 3.1. Comparison of SLAB and $D^2$ modeling approaches

In high RH environments, evaporative loss should be similar between each model because the relative humidity in the spray cloud is similar to the outside environment. By tuning the  $D^2$  model to match SLAB we can evaluate model differences as a basis to compare to drier environments. Downstream droplet mass fraction as predicted by the SLAB and  $D^2$  models for high RH is shown in Figure 1. Model agreement is within 10% in the near field (< 100 m) and within 30% in the far field (500 m). This is within reason and it is therefore reasonable to run each model for varying RH to determine influences of cloud processes on spray cloud dispersion.

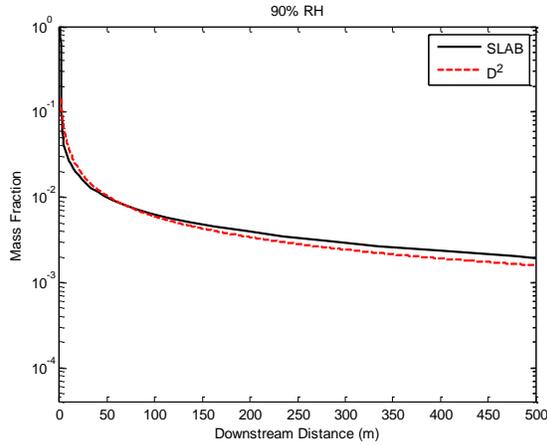


Figure 1. Comparison of SLAB and  $D^2$  models for a 90% relative humidity (dry bulb temperature = 300K).

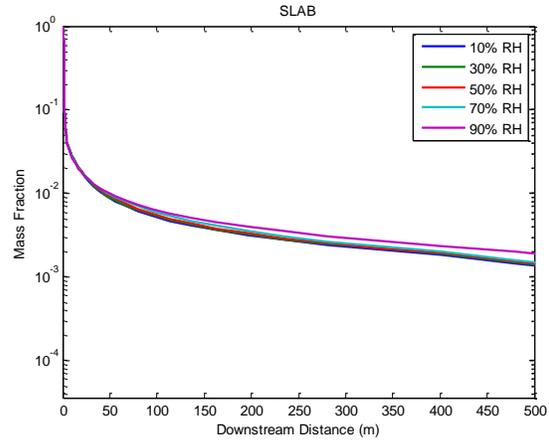


Figure 2. Mass fraction predictions from the SLAB model as a function of relative humidity (dry bulb temperature = 300K).

### 3.2. Sensitivity to relative humidity

To determine the relative sensitivity of each model to RH, we ran each model for varying RH from 10% to 70% with the same release and atmospheric characteristics described above. Each model predicts a decrease in droplet mass fraction in lower humidity environments (Figures 2 and 3). This is expected because droplet evaporation is higher in dryer environments. However, the  $D^2$  model is more sensitive to a decrease in RH as compared to the SLAB model. Because the models compare well for high RH, differences can be solely attributed to the lack of cloud effects in the  $D^2$  model. At 100 m downstream the difference between each model is less than a factor of two for  $RH > 30\%$ . However, at 500 m downstream the  $D^2$  model underpredicts mass fraction by over an order of magnitude as compared to the SLAB model. Over the first 500 m from the release, mean fractional error and mean fraction bias are listed in Table 1. Again, there is reasonable model agreement for high RH, however, the models diverge for low RH.

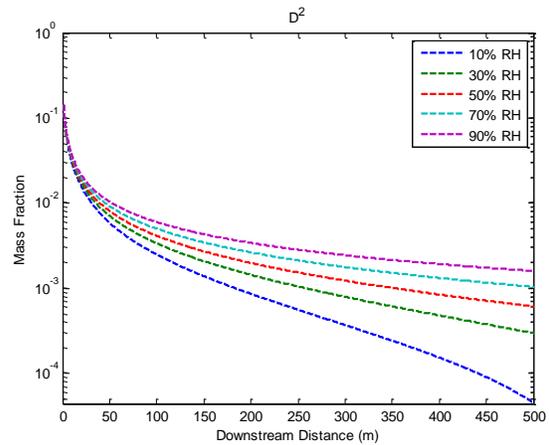


Figure 3. Mass fraction predictions from the  $D^2$  model as a function of relative humidity (dry bulb temperature = 300K).

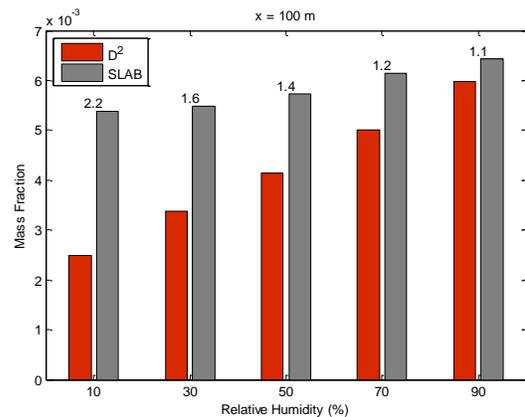
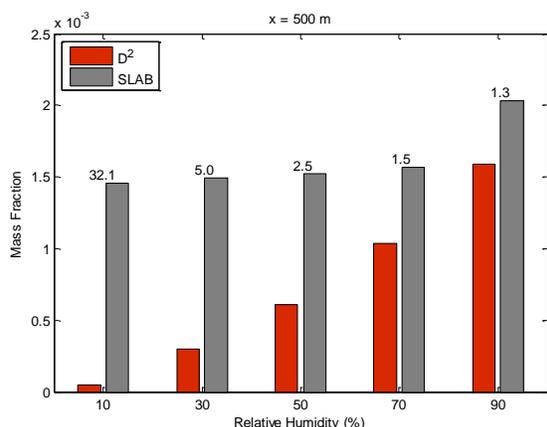


Figure 4. Mass fraction at 100 m from the source release as a function of relative humidity. Numbers above each bar group represents the difference factor between each model (i.e., SLAB /  $D^2$ ).



**Figure 5. Mass fraction at 500 m from the source release as a function of relative humidity. Numbers above each bar group represents the difference factor between each model (i.e., SLAB / D<sup>2</sup>).**

**Table 1. Mean fractional error (FE) and fractional bias (FB) between the SLAB and D<sup>2</sup> models over 500 m from the release as a function of RH.**

RH	10%	30%	50%	70%	90%
<b>FE</b>	6.46	1.72	0.79	0.33	0.13
<b>FD</b>	1.2	0.81	0.52	0.27	0.12

Often a general rule of thumb for dispersion studies is that within a factor of two agreement with observations is considered reasonable. Previous studies have evaluated dense gas models against a variety of source releases (e.g., Touma et al. 1995) and found within a factor of two agreement with observations. Similarly, AgDISP has replicated field observations by nearly a factor of 2 in the (Teske et al. 2011b). Holding to the factor of two logic, our results suggest droplet evaporation could cause significant model errors for RH < 30 within 100 m of the source release, and RH < 70% within 500 m from the source release. Therefore, this provides evidence that these effects should be treated more explicitly in applied spray drift models.

Incorporating cloud effects into current applied spray drift models may be challenging. Recent work involves defining an effective relative ambient humidity to capture cloud effects (Teske et al. 2011b). One drawback of this approach is that it may not be applicable over a wide range of spray and ambient conditions. Using a similar approach as dense gas models may provide some improvement for fine spray evaporation.

A caveat in this work is that we are assuming the SLAB model accurately represents dispersion of fine droplets from a steady source release. We are not aware of studies that evaluate dense gas models with field observations of fine pesticide spray droplets. Past experiments may not be ideal for evaluation of SLAB because of assumptions in gravitational settling or complex release configurations (e.g., Miller et al. 2000; Thistle et al. 2009). A detailed experiment on evaporative loss within spray clouds is needed to substantiate these findings.

#### 4. Conclusions

We used two disparate models to quantify potential evaporative loss errors in applied spray drift models. A dense gas model that captures thermodynamics effects of droplet evaporation was compared with a simple trajectory model that uses the D<sup>2</sup> law for droplet evaporation. Each model was compared for high RH and showed good agreement. However, for lower RH the models diverged up to over an order of magnitude at 500 m from the release. We attribute this to higher rates of droplet evaporation in the D<sup>2</sup> model.

These potentially large errors should be investigated further through additional experiments and model simulations. Future work should investigate evaporative loss under a wide range of spray and ambient conditions to identify periods where

evaporative loss may be highest. Improvements in applied spray drift model evaporation may be done similar approaches as dense gas models.

### Acknowledgements

This work was supported through a cooperative agreement with the USDA Forest Service.

### References

- Boutin, C., and B. Jobin, 1998: Intensity of agricultural practices and effects on adjacent habitats. *Ecol. Appl.*, **8**, 544–557, doi:10.2307/2641092.
- Davidson, C., and R. A. Knapp, 2007: Multiple stressors and amphibian declines: Dual impacts of pesticides and fish on yellow-legged frogs. *Ecol. Appl.*, **17**, 587–597, doi:10.1890/06-0181.
- Ermak, D. L., 1990: User's Manual for SLAB: An Atmospheric Dispersion Model for Denser-Than-Air Releases; UCRL-MA-105607.
- Felsot, A. S., J. B. Unsworth, J. B. H. J. Linders, G. Roberts, D. Rautman, C. Harris, and E. Carazo, 2011: Agrochemical spray drift; assessment and mitigation - A review. *J. Environ. Sci. Health Part B-Pestic. Contam. Agric. Wastes*, **46**, 1–23, doi:10.1080/03601234.2010.515161.
- Fettig, C. J., A. S. Munson, S. R. McKelvey, P. B. Bush, and R. R. Borys, 2008: Spray deposition from ground-based applications of carbaryl to protect individual trees from bark beetle attack. *J. Environ. Qual.*, **37**, 1170–1179, doi:10.2134/jeq2007.0300.
- Hanna, S., J. Chang, and D. Strimaitis, 1993: Hazardous Gas-Model Evaluation with Field Observations. *Atmospheric Environment Part a-General Topics*, **27**, 2265–2285, doi:10.1016/0960-1686(93)90397-H.
- Hanna, S., S. A. Abbasi, S. Dharmavaram, J. Zhang, I. Sykes, H. Witlox, S. Khajehnajafi, and K. Koslan, 2008: Comparison of six widely-used dense gas dispersion models for three recent chlorine railcar accidents. *Process Saf. Prog.*, **27**, 248–259, doi:10.1002/prs.10257.
- de Jong, A., J. M. G. P. Michielsen, H. Stallinga, and J. C. van de Zande, 2000: Effect of sprayer boom height on spray drift. *Mededelingen Faculteit Landbouwkundige en Toegepaste Biologische Wetenschappen Universiteit Gent*, **65**, 919–930.
- Miller, D. R., T. E. Stoughton, W. E. Steinke, E. W. Huddleston, and J. B. Ross, 2000: Atmospheric stability effects on pesticide drift from an irrigated orchard. *Trans. ASAE*, **43**, 1057–1066.
- Ramaprasad, J., M. Y. Tsai, K. Elgethun, V. R. Hebert, A. Felsot, M. G. Yost, and R. A. Fenske, 2004: The Washington aerial spray drift study: assessment of off-target organophosphorus insecticide atmospheric movement by plant surface volatilization. *Atmos. Environ.*, **38**, 5703–5713, doi:10.1016/j.atmosphere.2004.04.035.
- Schroeder, M., and D. Sturges, 1980: Spraying of Big Sagebrush with 2,4-D Causes Negligible Stream Contamination. *J. Range Manage.*, **33**, 311–312, doi:10.2307/3898081.

- Solomon, K. R., E. J. P. Marshall, and G. Carrasquilla, 2009: Human Health and Environmental Risks from the Use of Glyphosate Formulations to Control the Production of Coca in Colombia: Overview and Conclusions. *J. Toxicol. Env. Health Part A*, **72**, 914–920, doi:10.1080/15287390902929659.
- Teske, M. E., S. L. Bird, D. M. Esterly, T. B. Curbishley, S. L. Ray, and S. G. Perry, 2002: AgDRIFT (R): A model for estimating near-field spray drift from aerial applications. *Environ. Toxicol. Chem.*, **21**, 659–671, doi:10.1897/1551-5028(2002)021<0659:AAMFEN>2.0.CO;2.
- Teske, M. E., P. C. H. Miller, H. W. Thistle, and N. B. Birchfield, 2009: Initial Development and Validation of a Mechanistic Spray Drift Model for Ground Boom Sprayers. *Trans. ASABE*, **52**, 1089–1097.
- Teske, M. E. and Coauthors, 2011a: A Review of Computer Models for Pesticide Deposition Prediction. *Trans. ASABE*, **54**, 789–801.
- Teske, M. E., H. W. Thistle, and R. J. Londergan, 2011b: Modification of Droplet Evaporation in the Simulation of Fine Droplet Motion Using Agdisp. *Trans. ASABE*, **54**, 417–421.
- Thistle, H. W., 2000: The role of stability in fine pesticide droplet dispersion in the atmosphere: A review of physical concepts. *Trans. ASAE*, **43**, 1409–1413.
- Thistle, H. W., G. G. Ice, R. L. Karsky, A. J. Hewitt, and G. Dorr, 2009: Deposition of Aerially Applied Spray to a Stream Within a Vegetative Barrier. *Trans. ASABE*, **52**, 1481–1490.
- Touma, J., W. Cox, H. Thistle, and J. Zapert, 1995: Performance Evaluation of Dense Gas Dispersion Models. *J. Appl. Meteorol.*, **34**, 603–615, doi:10.1175/1520-0450(1995)034<0603:PEODGD>2.0.CO;2.
- Trayford, R. S., and L. W. Welch, 1977: Aerial Spraying a Simulation of Factors Influencing the Distribution and Recovery of Liquid Droplets. *Journal of Agricultural Engineering Research*, **22**, 183–196.
- Ward, M. H. and Coauthors, 2006: Proximity to crops and residential exposure to agricultural herbicides in Iowa. *Environ. Health Perspect.*, **114**, 893–897, doi:10.1289/ehp.8770.