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A Comparison of Ammonia Emission Rates from an Agricultural Area Source Using Dispersion Modeling: Gaussian versus Backward-Lagrangian Stochastic

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Abstract. *Agricultural operations are thought to contribute significantly to the overall anthropogenic ammonia emissions. Ammonia emissions serve as crucial elements of atmospheric models because ammonia is one of the most prevalent alkaline gaseous bases found in the planetary layer. Ammonia concentrations affect the overall acidity of precipitation and atmospheric aerosols. These ammonia aerosols have the attention of the EPA and other regulatory agencies because, when certain thresholds are exceeded, potential consequences result from these over-threshold concentrations of oxidized and reduced forms of nitrogen.*

In this study, an evaluation of ammonia emission rates generated by both the Industrial Source Complex (Gaussian) model and the WindTrax (backward-Lagrangian stochastic) model revealed that the calculated emission concentrations from each model using the average emission rate generated by the model vary by a factor of 10.

Current and future sources are regulated by the emission rate data from previous time periods. Emission factors are published for regulation of various sources, and these emission factors are derived based upon back-calculated model emission rates and site management practices. Thus, a factor of 10 ratio in the emission rates could prove troubling in terms of regulation if the model that the emission rate is back-calculated from is not used as the model to predict a future downwind pollutant concentration.

Keywords. Aerosols, Air Pollution, Air Quality, Air Sampling, Ammonia, Backward Lagrangian Stochastic, Dispersion Modeling, Emission Rate, Gaussian, Regulatory Compliance, Regulatory Policy

Introduction

Ammonia (NH_3) emissions serve as crucial elements of atmospheric models because ammonia is one of the most prevalent gaseous bases found in the planetary boundary layer (PBL). Ammonia concentrations affect the overall acidity of precipitation, cloud water, and atmospheric aerosols (Aneja et al., 2001). Typically, ammonia reacts with acidic species to form ammonium sulfate ($(NH_4)_2SO_4$), ammonium nitrate (NH_4NO_3), ammonium chloride (NH_4Cl), ammonium and the hydroxyl radical (NH_4^+ and OH^-), or it may be deposited to the earth's surface by either dry or wet deposition processes (Seinfeld and Pandis, 1998).

Ammonia atmospheric aerosols have the attention of the EPA and other regulatory agencies because these aerosols are thought to comprise a large part of secondary $PM_{2.5}$, which is a classification for particulate matter with an aerodynamic equivalent diameter less than or equal to a nominal 2.5 μm (Makar et al., 2003; Gupta et al., 2003; Aneja et al., 2001; Yamamoto et al., 1988; Battye et al., 1994). Secondary pollutants result from the chemical reaction among two or more pollutants. Researchers have shown that a large percentage of $PM_{2.5}$ penetrates human respiratory systems and deposits in the lungs and alveolar region, subsequently endangering the public health (Hinds, 1999; Aneja et al., 2001). Additionally, these atmospheric aerosols have the potential to significantly influence global warming and ozone depletion and to cause major environmental damage when redeposited on land and water (MAFF, 1998).

Currently, neither the EPA nor the Texas Commission of Environmental Quality (TCEQ) regulates ammonia as a criteria pollutant. However, ammonia concentration levels are monitored by Effects Screening Levels (ESLs). If airborne ammonia concentration ESLs are not exceeded, then negative health effects and/or welfare effects would not be anticipated (TNRCC, 2001). However, ammonia emissions are now being considered as an air quality concern. Literature notes that agricultural operations account for a considerable amount of the anthropogenic ammonia emitted (Battye et al., 1994; Aneja et al., 2003; Arogo et al., 2001). Subsequently, ammonia emissions from agricultural operations have drawn attention from the regulators and the agricultural industry as well as the general public outside of the agricultural industry. An understanding of the transport and modeling of NH_3 and the inherent error surrounding the modeling process is essential for appropriate regulatory decisions and determination of source compliance with future regulatory policy.

In order to determine ESL exceedances, ammonia emissions must be quantified appropriately. Gas sampling from an industrial process can be easily performed by directly sampling from the stack exhaust. However, it is much more challenging to quantify gaseous emissions from an area source. One option is to utilize atmospheric dispersion modeling to back-calculate pollutant emission rates indirectly. Literature notes that the backward modeling approach offers a lot in terms of ease of calculations, efficiency, and flexibility (Flesch et al., 1995).

This research evaluates the results of two dispersion models to back-calculate the emission rate of ammonia from an area source. To perform this back-calculation, a Gaussian Plume dispersion model, ISC-ST3 (Industrial Source Complex – Short Term Version 3), with the Breeze user interface (Trinity Consultants, 12801 N. Central Exp., Suite 1200, Dallas, TX, 75243), was evaluated and compared to a backward-Lagrangian stochastic based model, WindTrax, (Thunder Beach Scientific, 4B-1127 Cartaret Street, Halifax, Nova Scotia, Canada, BH3 3P2). Equivalent test data was input into each dispersion model for comparison of back-calculated emission rates.

Air Pollution Dispersion Modeling

Modeling of air pollutants plays an important role in the regulatory process by mathematically and scientifically describing the causal relationship between pollutant emissions and corresponding atmospheric concentrations (Builtjes, 2003). Dispersion models provide a means to mathematically simulate the transport of gases and particles through the atmosphere. Estimates of pollutant concentrations downwind of a source can be established from the pollutant emission rate and the meteorological conditions using a defined mathematical model. Part of the state regulatory process includes demonstrating compliance with air quality standards for all regulated pollutants. Dispersion modeling provides a scientific method for the regulatory agency to measure air quality compliance of a future source (one that has not been constructed). Additionally, dispersion modeling can be utilized to quantify the impact of a change in an abatement strategy of an existing source (Builtjes, 2003).

Gaussian Dispersion Modeling

Currently, the EPA has approved Industrial Source Complex – Short Term 3 (ISC-ST3) as the short range dispersion model used to model low level sources, such as animal feeding operations (40 CFR Part 51, 1999). This model is based on a double reflected Gaussian dispersion model, which describes the horizontal and vertical concentration distributions with the assumptions of continuous emissions, conservation of mass, steady-state conditions, and normal distribution of crosswind and vertical concentrations of pollutants (Cooper and Alley, 2002). The Gaussian dispersion model utilizes the experimentally determined Pasquill-Gifford horizontal and vertical plume spread parameters, σ_y and σ_z as seen in equation 1 below.

$$C_{10} = \frac{Q}{2\pi u \sigma_y \sigma_z} \exp\left(-\frac{1}{2} \frac{y^2}{\sigma_y{}^2} \right) \left\{ \exp\left(-\frac{1}{2} \frac{(z-H)^2}{\sigma_z{}^2} \right) + \exp\left(-\frac{1}{2} \frac{(z+H)^2}{\sigma_z{}^2} \right) \right\} \quad [1]$$

where C_{10} is the 10 minute concentration (μg/m^3), Q is the emission rate (μg/s), u is the one hour average wind speed at stack height (m/s), y is the horizontal distance from the centerline of the plume (m), z is the height of the receptor with respect to the ground level (m), and H is the effective stack height (m) (Cooper and Alley, 2002). Using measured concentration values as well as meteorological data from the concentration sampling period, a pollutant emission rate can be back-calculated through equation 1.

Backward Lagrangian Stochastic (bLS) Modeling

Lagrangian stochastic (LS) models, also known as random-flight models, determine particle trajectories in attempt to imitate turbulent dispersion. By simulating individual parcels of air, the LS model predicts the path followed by each parcel to reach a receptor (Seinfeld and Pandis, 1998).

The bLS model is based on the forward LS model, which is the generalized Langevin equation under the assumption that the position of a particle evolves jointly as a Markov process with the velocity (Flesch et al., 1995). This model by Flesch, which is simulated by the WindTrax software, accounts for the location of particle impact with the ground and the subsequent reflection of these particles back into the atmosphere.

The model uses this information to define the ratio of the modeled concentration to the emission rate $(C/Q)_{sim}$ as seen in equation 2 below (Flesch et al., 2004a).

$$(C/Q)_{sim} = \frac{1}{N}\Sigma\left|\frac{2}{w_0}\right| \qquad [2]$$

where N is the number of particles and w_o are the vertical touchdown velocities at the particle's impact with the ground. The bLS model requires the specification of wind statistics for the surface layer. These can be calculated using established Monin-Obukhov similarity theory (MOST) based formulas (Flesch et al., 2004a). The MOST approach asserts that the average gradient and turbulent features of a stratified surface layer only rely upon the height, the kinematic heat flux, the buoyancy variable, and the kinematic surface stress (Arya, 2001).

The bLS approach is based on simulating atmospheric diffusion at a specific location, and its validity hinges upon the fundamental diffusion and subsequent Lagrangian models. The air parcels simulated by the Lagrangian model are vertical columns of air that extend from the ground up to some height *H* (Seinfeld and Pandis, 1998). An underlying assumption in the Lagrangian trajectory model is that, when applied to reacting species, it is only applicable to linearly reactive species (Lamb and Seinfeld, 1973). An additional underlying assumption is that the chemical reactions that occur are independent of particle displacement and are not determined by the frequency of the collisions of particles (Lamb and Seinfeld, 1973). First the three-dimensional wind field, which is defined by $u_x(x, y, z)$, $u_y(x, y, z)$, and $u_z(x, y, z)$, is used to calculate the backward trajectories of the air parcels from equation 3 (Seinfeld and Pandis, 1998):

$$\frac{d\vec{s}(t)}{dt} = \vec{u}(t) \qquad [3]$$

where the location of the air parcel at time *t* is $\vec{s}(t)$ and $\vec{u}(t)$ is the wind velocity vector (defined by u_x, u_y, u_z). If this equation is integrated from *t* to t_o, then the location of the air parcel at any given time *t* on the backward trajectory of the particle, which is defined by $\vec{s}(t)$, can be calculated straightforwardly as:

$$\vec{s}_0 - \vec{s}(t) = \int_t^{t_o} \vec{u}(\tau)d\tau \qquad [4]$$

assuming that at a time t_o the trajectory ends at the location $\vec{s}_0$. Following the calculation of the trajectory path $\vec{s}(t)$, corresponding emission fluxes can be determined by interpolating the emission field *E* (*x, y, z, t)* and defining flux along the trajectory path, $E_t(t)$ as (Seinfeld and Pandis, 1998):

$$E_t(t) = E(\vec{s}(t), t) \qquad (5)$$

The basic diffusion equation is built upon the basic continuity assumption

$$\frac{\partial c_i}{\partial t} + u_x\frac{\partial c_i}{\partial x} + u_y\frac{\partial c_i}{\partial y} + u_z\frac{\partial c_i}{\partial z} = \frac{\partial}{\partial x}\left(K_{xx}\frac{\partial c_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{yy}\frac{\partial c_i}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_{zz}\frac{\partial c_i}{\partial z}\right) + R_i(c_1, c_2, \ldots, c_n) + E_i(x, y, z, t) - S_i(x, y, z, t) \qquad [6]$$

for i = 1, 2, …N, where c_i denotes the theoretical mean concentration of species i, K represents the corresponding eddy diffusivity components, R_i is the chemical generation of species *i*, E_i describes the emission flux, S_i is the removal flux, and *u* represents the mean value for each of

the wind velocity components. Equation 6 can be simplified to correspond to a coordinate system that moves horizontally with velocities equal to the wind speed. Thus, the particle moves at a velocity equal to that of the wind speed, and no material exchange exists between the parcel and its surroundings by advection (Seinfeld and Pandis, 1998). Thus, the diffusion equation can be simplified to

$$\frac{\partial c_i}{\partial t} + u_z \frac{\partial c_i}{\partial z} = \frac{\partial}{\partial x}\left(K_{xx} \frac{\partial c_i}{\partial x} \right) + \frac{\partial}{\partial y}\left(K_{yy} \frac{\partial c_i}{\partial y} \right) + \frac{\partial}{\partial z}\left(K_{zz} \frac{\partial c_i}{\partial z} \right) + R_i\left(c_1, c_2, ..., c_n\right) + E_{t,i}(t) - S_i(t) \quad [7]$$

The diffusion equation can be further simplified in the local model by comparing the vertical advective transport, which is described by the term $u_z \frac{\partial c_i}{\partial z}$, to the vertical turbulent dispersion, which is described by the term $\frac{\partial}{\partial z}\left(K_{zz} \frac{\partial c_i}{\partial z} \right)$ in the diffusion equation (Seinfeld and Pandis, 1998). This assumption can be written as:

$$\left| u_z \frac{\partial c_i}{\partial z} \right| << \frac{\partial}{\partial z}\left(K_{zz} \frac{\partial c_i}{\partial z} \right) \quad [8]$$

Thus, the $u_z \frac{\partial c_i}{\partial z}$ term can be neglected in the diffusion equation. Next, assuming that horizontal concentration gradients contribute negligibly to the overall mass balance of the system, the horizontal turbulent dispersion terms can be neglected (Seinfeld and Pandis, 1998). Note, this assumption contributes a very small error in an area with homogenous emissions (uniform emission across the source); however, the error from this assumption becomes quite important in an area dominated by a few strong point sources (Seinfeld and Pandis, 1998). These two assumptions can be stated as:

$$\frac{\partial}{\partial x}\left(K_{xx} \frac{\partial c_i}{\partial x} \right) \cong 0 \quad \text{and} \quad \frac{\partial}{\partial z}\left(K_{zz} \frac{\partial c_i}{\partial z} \right) \cong 0 \quad [9]$$

The third and final, simplifying assumption to the diffusion equation is to neglect the wind shear. The Lagrangian model assumes that the air column being modeled remains intact during transport, thus assuming that

$$u_x(x, y, z, t) \cong u_x(x, y, t) \quad [10]$$

and

$$u_x(x, y, z, t) \cong u_x(x, y, t) \quad [11]$$

Literature notes that this assumption is critical to the validity of the trajectory model (Liu and Seinfeld, 1975). Additionally, literature notes that this provides a major source of error in some of the trajectory model calculations, in particular those models that utilize long transport times.

With these three assumptions, the one dimensional Lagrangian trajectory model, a simplification of the initial diffusion equations, can be written as

$$\frac{\partial c_i}{\partial t} = \frac{\partial}{\partial z}\left(K_{zz} \frac{\partial c_i}{\partial z} \right) + R_i\left(c_1, c_2, ..., c_n\right) + E_{t,i}(t) - S_i(t) \quad [12]$$

Assuming that the source is continuously emitting and homogenous turbulence, a Gaussian plume becomes the solution to the Lagrangian equation. However, even in nonstationary and inhomogenous turbulence, the Gaussian equation can give an estimate of reasonable order of magnitude in practical circumstances (Lamb and Seinfeld, 1973).

The backward – Lagrangian model used by Flesch et al. (2004b) is based on the simplified Lagrangian equation and of assumptions. However, literature from these scientists notes that the backward model accounts for particle reflection from the surface, as does the Gaussian model used in this evaluation, which leads to false particle gradients at the surface (Flesch et al., 1995). To reduce this error potential, the time scale on the model is reduced, thus reducing the maximum source to receptor distance of the model. Research has shown that the backward model is about 50 times faster than the forward LS model when predicting concentrations from a substantial area source at a short range (Flesch et al., 1995). The bLS model utilizes touchdown catalogs to determine the source of the particles arriving to a receptor location.

The touchdown catalogs are independent of the average wind speed and concentration data, so, the model can be initially run without knowledge of the source geometry (Flesch et al., 2004b). Inherent in the bLS model are the same essential assumptions of the LS model: horizontally homogenous flow and a spatially uniform emission rate of the species being modeled (Flesch et al., 2004a).

Dispersion Modeling Inputs Defined

Back-calculated ammonia emission rates from concentration and meteorological field condition data were used to compare the two models. Identical meteorological and concentration data for each test period were used in both models to determine the average emission rate for each respective test period. The actual meteorological data used in this comparison can be obtained from the authors if needed.

Receptor Layout

Figure 1 describes the basic layout of Feedyard C and the location of the passive ammonia samplers. Seven passive samplers (receptors), which are depicted by red on Figure 1, were placed along the downwind fence line of the feedyard. Additionally, a tower was placed at a location halfway down the width of the feedyard, and receptors were placed at three different heights along this tower: 1.5 m, 3 m, and 6 m.

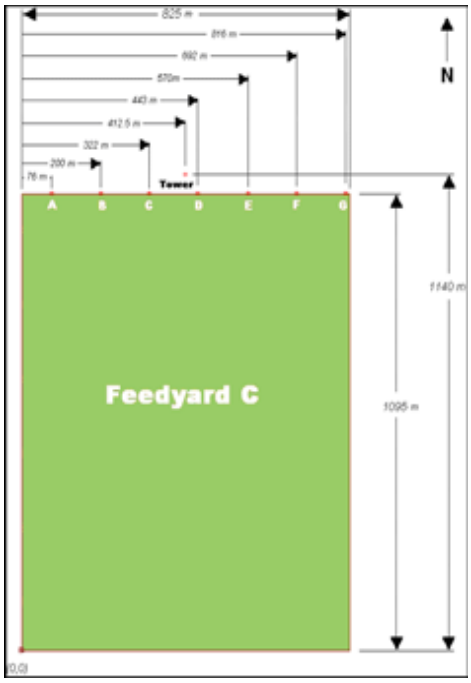

Figure 1. Ammonia Receptor Feedyard Layout.

Meteorological Inputs

The stability of the atmosphere was the only input that was not directly measured by a sensor and was determined based on other data. Atmospheric stability was described using the Pasquill-Gifford parameters where A corresponded to very unstable conditions, B corresponded to moderately unstable conditions, C corresponded to slightly unstable conditions, D corresponded to neutral conditions, E corresponded to slightly stable conditions, and F corresponded to stable conditions (Cooper and Alley, 2002). These stability classes were determined using the Solar Radiation Delta-T (SRDT) Method for Estimating the Pasquill-Gifford Stability Class from the *Meteorological Monitoring Guidance for Regulatory Modeling Applications* published by the EPA and used in regulatory compliance monitoring, which can be seen in Table 1 (US EPA, 2000). The SRDT method requires the surface layer wind speed, the daytime solar radiation measurements, and the nighttime vertical temperature gradients measured at the sampling location as data inputs. The basic rationale of Turner's method, which provides an initial way to determine the Pasquill-Gifford stability classes from National Weather Service data, supplies the foundation for the SRDT method (Turner, 1964). However, the SRDT method accounts for the time periods with cloud cover and ceiling (US EPA, 2000). With the weather data, daytime stability classes were determined easily based from the solar radiation value and the wind speed. However, during the data collection period, nighttime vertical temperature gradients were not available. Since the ammonia concentration data was collected in August, 2002, it was assumed that the vertical temperature gradient was less than zero (the temperature of the local air decreases as the height increases). The atmospheric data indicated that in the evening hours, the soil temperature was greater than the air temperature above the soil, so this assumption was valid at the surface, and it was assumed that this trend continued as the height increased.

Table 1. SRDT Method for Estimating Stability Class. (adapted from US EPA, 2000)

Daytime				
Wind Speed (m/s)	Solar Radiation (Watts/m^2)			
	≥ 925	925 – 675	675 – 175	< 175
< 2	A	A	B	D
2 – 3	A	B	C	D
3 – 5	B	B	C	D
5 – 6	C	C	D	D
≥ 6	C	D	D	D
Nighttime				
Wind Speed (m/s)	Vertical Temperature Gradient			
	< 0		≥ 0	
< 2.0	E		F	
2.0 – 2.5	D		E	
≥ 2.5	D		D	

Back-Calculated Emission Rate

With all of the input data defined, the average back-calculated emission rate for each test was determined using the two different dispersion models: ISC-ST3 (Gaussian based) and WindTrax (backward-Lagrangian based).

Gaussian Plume Dispersion Model

The Gaussian plume based dispersion model Industrial Source Complex – Short Term version 3 (ISC-ST3) is recommended by the EPA for industrial sources, rural or urban areas, flat or rolling terrain, transport distances less than 50 kilometers, one-hour to annual averaging times, and continuous toxic air emissions (Trinity Consultants, 2000). Thus, it was appropriate to model an agricultural operation such as Feedyard C using this model.

For the Gaussian Plume based dispersion model, ISC-ST3 was used with the Breeze user interface. The method used in this analysis to back-calculate emission rates from the area source is the method used by researchers from the Center for Agricultural Air Quality Engineering and Science at Texas A&M University.

The ISC-ST3 model was graphically built with the feedyard layout and receptor layout as shown in Figure 1. The ISC-ST3 layout can be seen in Figure 2. By going into the data screen on ISC, an emission rate for the area source was set at $6*10^{-6}$ g/m^2/s, and the start and stop test times were specified. Next, a meteorological file was built using the MetView add-in and inputting the hourly wind speed, wind direction, and stability class information as measured at the feedyard. This file was then linked as the meteorological data for the model. Note that the ISC model assumes a constant wind vector field across the entire area source for the hourly time period. Further information on running the ISC-ST3 application (Breeze Interface) can be obtained from the Center for Agricultural Air Quality Engineering and Science or Trinity Consultants (CAAQS, 2004; Trinity Consultants, 2000).

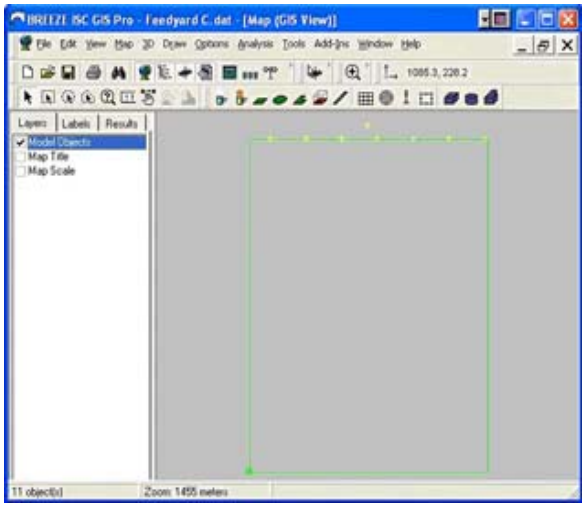

Figure 2. ISC Layout Screen Shot.

With the input data established, the ISC model was run. The governing equation for the ISC model is the Gaussian equation as noted in equation 1. This equation shows the direct relationship that exists between the concentration (C) and the emission rate (Q). As C is increased by a factor of x, Q is also increased by a factor of x. Thus, by defining the initial emission rate guess into ISC-ST3 ($6*10^{-6}$ g/m^2/s) as Q_1 and the output concentration at a receptor as C_1, the actual net measured concentration, C_2, can be used to find the emission rate, Q_2, needed to generate this concentration at receptor *i* based off of the relationship in equation 13.

$$\left(\frac{C_1}{Q_1}\right)=\left(\frac{C_2}{Q_2}\right) \qquad [13]$$

which can be rewritten as

$$Q_2=\left(\frac{C_2}{C_1}\right)*Q_1 \qquad [14]$$

Because the passive samplers were located on the same fence line of the feedyard, no single more downwind sampler exists. Therefore, an average was taken from these 10 receptor emission rate calculations to determine the average emission rate for the test period. Using the same conceptual equation as in 13 and the ISC-ST3 model, this emission rate was used to predict the pollutant concentration at each receptor location had the average emission rate been used with the same input data (with the predicted concentration as C_2 and the average emission rate as Q_2 as seen below in equation 15).

$$C_2=\left(\frac{Q_2}{Q_1}\right)*C_1 \qquad [15]$$

This process was performed for each set of test data. Table 2 shows the average back-calculated emission rates for each of the test periods.

Table 2. Average Calculated Emission Rates Using ISC-ST3.

Test #	ISC ER g/(m^2-s)	Test Length (hrs)	Stability Classes in this Test
111	8.66E-06	2	D, C
112	1.03E-05	3	C, B, C
113	6.68E-06	3	All D
114	4.64E-06	12	All D
121	3.60E-06	7	D,D,D,D,D,D,C
122	7.62E-06	5	All D
123	5.31E-06	12	All D
131	6.03E-06	3	All D
132	1.03E-05	3	All D
133	1.05E-05	3	All D
134	7.17E-06	3	All D
135	4.47E-06	12	All D
141	4.42E-06	3	D, D, C
142	3.90E-06	3	C, C, B
143	7.06E-06	3	All B
144	8.14E-06	3	C, C, D
145	2.98E-06	12	All D
151	6.56E-06	3	All D
152	7.53E-06	3	C, C, B
153	1.14E-05	3	B, C, C
154	8.15E-06	3	All D
155	2.48E-06	12	D, D, D, D, E, E, E, E, E, D, D, D

Backward Lagrangian Stochastic (bLs) Model

The backward Lagrangian Stochastic model is a local dispersion model (it should be used for short term modeling, not long term modeling). Since regulatory monitoring to comply with regulations such as the NAAQS is performed near the source, this model may be applied. Additionally, the relatively flat surface of the rural environment provides a perfect emission surface of the Lagrangian trajectory model.

For this part of the analysis, Windtrax (Version 1.0, Release 1.4.2, Thunder Beach Scientific, Alberta, Canada) was utilized as the backward-Lagrangian stochastic model. The user's guide notes that this model is restricted to ground level sources only (elevated sources are not possible with this algorithm), and the source to receptor distances must be less than about 1 km (Thunder Beach Scientific, 2003). The source to receptor distances in the feedyard example were about 1.1 km apart, which was at the upper boundary of the valid source to receptor distance. Additionally, it states that WindTrax 1.0 is only valid where the source is bare ground (or short vegetation), and the wind blows undisturbed (Thunder Beach Scientific, 2003).

Before proceeding with the evaluation of the bLs model, it is important to restate the underlying assumptions as described in the literature review (Liu and Seinfeld, 1975). First, the coordinate system is defined as a moving coordinate system that moves horizontally with velocities equal to the wind speed thus eliminating advection, which is the standard assumption of trajectory

models. Second, horizontal diffusion is neglected by assuming that the horizontal concentration gradients contribute negligibly to the overall mass balance of the system. Third, the vertical wind component has been ignored, thus assuming that air parcel movement is two-dimensional. Finally, the wind shear is neglected because the Lagrangian model assumes that the column height of the air parcel remains intact throughout the trajectory. The backward-Lagrangian model is a modified version of the original Lagrangian model in order to account for the touchdown of particles at various locations on the source surface. Thus, the assumptions of the bLS model are horizontally homogenous flow and a spatially uniform emission rate of the modeled species (Flesch et al., 1995).

Pre-modeling Tests

Before the model was run, various tests were used to determine how the bLS model functions because the actual source code for this particular model is not in the public domain unlike the ISC Gaussian model. The modeling procedure will be detailed in the following section.

First, the reversibility of the model was tested. Using the receptor layout at the feedyard as shown in Figure 6.1, a random emission rate (6 $\mu g/m^2/s$) was used to generate concentration data at each receptor for a given set of meteorological data. Then, the emission rate was set as unknown and calculated from the same given set of meteorological and previously generated concentration data. The calculated emission rate (6.07 $\mu g/m^2/s$) was within 1% of the original emission rate. This error was most likely attributed to a rounding error. The calculated concentrations for each receptor was rounded when re-input into the model. This alone could cause the 1% difference. Thus, the reversibility of the model was affirmed.

Next, the relationship between the emission rate and the concentration at the receptor was verified. A simplified plot was used with a single area source and single concentration receptor with an unknown concentration. The emission rate was set at 10 $\mu g/m^2/s$, and the receptor concentration was calculated to be 67.9 $\mu g/m^3$. Then, the emission rate was multiplied by a factor of 2 to 20 $\mu g/m^2/s$, and the receptor concentration was calculated to be 136 $\mu g/m^3$. Thus, the concentration at the receptor was also increased by a factor of 2 when the emission rate was increased by the same factor. The emission rate was then multiplied by a factor of 3, 4, and 5, and the receptor concentration increased by a factor of 3, 4, and 5, respectively. Therefore, it can be said that a directly proportional relationship exists between the species emission rate and the concentration of that species at a downwind receptor.

In order to use the ammonia concentration data collected over a time period longer than that of the meteorological data and to ensure that the models are being compared in the same way, the bLS model was used to back-calculate the emission rate in the same way as the ISC-ST3 model. A random emission rate is used to generate concentration values at each receptor for each hour of meteorological data. Then, an emission rate necessary to calculate this receptor concentration was calculated by utilizing the proportional relationship that exists between the emission rate and the concentration at the receptor. For comparison purposes, an average emission rate was computed from the ten calculated emission rates. The process of determining these values in the bLS model is discussed in the next subsection.

Determination of the Area Emission Rate

The process for back-calculating an emission rate in the bLS model is different than that of the ISC (Gaussian) model, but the inputs are the same. In order to back-calculate an emission rate for an area source in the bLS model, the user must input the following parameters:

1. Coordinates of the area source
2. Wind speed at the main anemometer
3. Wind direction at the main anemometer
4. Height of the main anemometer
5. Atmospheric stability (in terms of Pasquill-Gifford Stability Class, Monin-Obukhov length, general stability condition description, present weather conditions, or the gradient Richardson number)
6. Pollutant background concentration at a receptor
7. Height of the receptor
8. Coordinate location of each receptor
9. Soil surface data

Using the same input data as the ISC-ST3 (Gaussian based model), the Windtrax (bLS based model) was run. Concentration receptors were placed at a 3.0 m height along the fence line at 76 m, 200 m, 322 m, 443 m, 570 m, 692 m, and 816 m. Additionally, a tower was placed at (412.5 m, 1140 m) with concentration receptors placed at 1.5 m, 3 m, and 6 m. All 10 concentration receptors in the model were set in the unknown mode of the sensor output by clicking on the unknown option under the "Measurement" tab of the concentration sensor window. For the comparison in this research an emission rate of 6 $\mu g/m^2/s$ was input as uniform across the drawn area source and was used to determine relative concentrations at each receptor. The Windtrax layout can be seen in Figure 3 that follows.

With all of the inputs to the model specified, the model was run using the green arrow at the top of the screen. While the model ran, the individual backward particle trajectories were seen as a series of red dots on the model as seen in two different tests in Figure 4.

After the model completed its run, the created output file was accessed to see the concentration data generated by the bLS model for a given emission rate. This information was then used to calculate the average emission rate for a test period.

When the model ran with the current feedyard conditions, a warning was generated because the source to receptor distance (noted as the tracking distance in the model output) exceeded the 1 km specified maximum distance. The length of the feedyard was 9.5% over this maximum distance (1.095 km). The user's guide notes that the analysis of this model is restricted to source to receptor distances of less than about 1 km (Thunder Beach Scientific, 2003). Within a reasonably small error, the source to receptor distance in the model was at the upper boundary of the source to receptor distance considered to be valid to run the model.

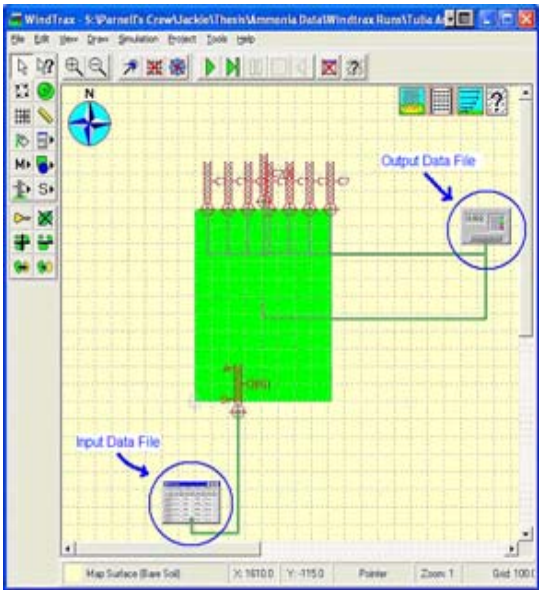

Figure 3. Screen Shot of the BLS Prior to Running the Model.

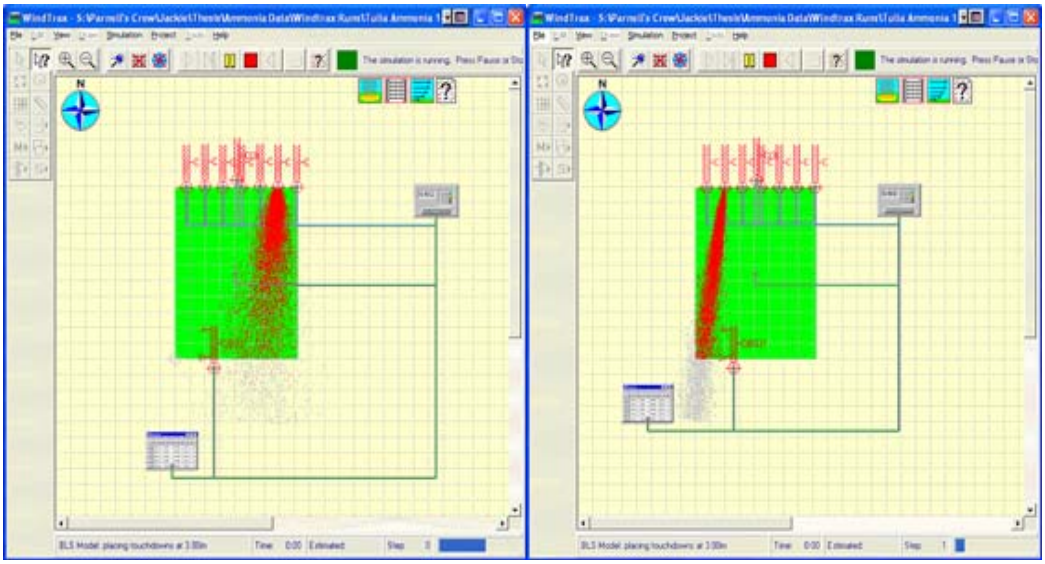

Figure 4. Examples of the BLS Model During 2 Different Runs.

In order to ensure that the same outputs were being compared, the WindTrax model was run the same manner as ISC-ST3 in order to back-calculate an emission rate from the feedyard area source. This method was followed because the ammonia concentration data used was over a larger time frame than the relatively small Δt between concentration measurements assumed by the bLS model. So, a method similar to that used in determining the average emission rate for a time period with the ISC model was employed. Each test ran with the previously described layout, parameters, and a standard emission rate of 6 $\mu g/m^2/s$. The bLS model was used to calculate pollutant concentrations at each of the input receptors with the given meteorological data and standard emission rate. For comparison purposes, the emission

rate necessary to achieve a given concentration at a receptor was calculated in the exact same manner as the ISC model method previously described using equation 13.

Equation 13 shows the direct relationship that exists between the concentration (C) and the emission rate (Q), and the pre-modeling tests verify the validity of using this directly proportional relationship of C and Q. As C increased by a factor of x, Q also increased by a factor of x. Thus, by defining the initial emission rate guess into the bLS model, Windtrax, ($6*10^6$ g/m^2/s) as Q_1 and the output concentration at a receptor as C_1, the actual net measured concentration, C_2, was used to find the emission rate, Q_2, needed to generate this concentration as in equation 14. As previously done in the ISC model calculations, an average of the 10 receptor emission rate calculations was used to determine the average emission rate for the test period. This was done because no single more downwind sampler existed since the passive samplers were located on the same fence line of the feedyard. Using equation 15, the emission rate was used to generate the bLS predicted concentration at the receptor location had the average emission rate been used with the same input data (with the predicted concentration as C_2 and the average emission rate as Q_2).

This emission rate back-calculation process was performed for each set of test data. Table 3 shows the average emission rate results of the bLS analysis for each of the test periods. With the average emission rates for each test calculated, the bLS model results were in a form that could be easily compared to the Gaussian model results.

Table 3. Average Calculated Emission Rates Using WindTrax.

Test #	bLS ER g/m^2/s	Test Length (hrs)	Stability Classes
111	9.05E-05	2	D, C
112	1.03E-04	3	C, B, C
113	6.99E-05	3	All D
114	4.84E-05	12	All D
121	3.64E-05	7	D,D,D,D,D,D,C
122	9.09E-05	5	All D
123	5.57E-05	12	All D
131	6.31E-05	3	All D
132	1.08E-04	3	All D
133	1.08E-04	3	All D
134	7.55E-05	3	All D
135	4.67E-05	12	All D
141	4.67E-05	3	D, D, C
142	3.53E-05	3	C, C, B
143	5.68E-05	3	All B
144	8.22E-05	3	C, C, D
145	3.14E-05	12	All D
151	6.51E-05	3	All D
152	7.24E-05	3	C, C, B
153	1.13E-04	3	B, C, C
154	8.56E-05	3	All D
155	1.86E-05	12	D, D, D, D, E, E, E, E, E, D, D, D

Model Output Discussion

After running the Gaussian based ISC-ST3 model and the backward Lagrangian Stochastic based WindTrax models, the outputs can be compared. The average emission rate for each test as computed by each model were computed in a way to ensure that the model inputs are the same. Table 4 summarizes the comparison of the emission rates from the two models evaluated in this research: the EPA regulatory approved ISC-ST3 Gaussian based dispersion model and the backward-Lagrangian Stochastic based WindTrax model. The first column of Table 4 indicates the test number of the data. The second column shows the emission rate generated by the ISC model (Gaussian based). The third column displays the emission rate generated by the WindTrax model (bLS based). The forth column calculates the difference between the bLS model and the ISC model. The next column computes the order of magnitude difference between the emission rates generated in each model (it is the bLS back-calculated emission rate divided by the ISC back-calculated emission rate).

Table 4. Overall Comparison of Summary Model Outputs.

Test #	ISC ER	bLS ER	Diff	Factor (bLS/ ISC)	Day/ Night	Δt	Stability Classes
	μg/m^2/s	μg/ m^2/s	μg/ m^2/s			(hrs)	
111	8.66	90.5	81.9	10.46	Day	2	D, C
112	10.3	103	93.1	10.06	Day	3	C, B, C
113	6.68	69.9	63.3	10.47	Day	3	All D
114	4.64	48.4	43.7	10.43	Night	12	All D
121	3.60	36.4	32.8	10.11	Day	7	D,D,D,D,D,D,C
122	7.62	90.9	83.2	11.93	Day	5	All D
123	5.31	55.7	50.3	10.49	Night	12	All D
131	6.03	63.1	57.1	10.46	Day	3	All D
132	10.3	108	97.5	10.43	Day	3	All D
133	10.5	108	97.4	10.25	Day	3	All D
134	7.17	75.5	68.3	10.53	Day	3	All D
135	4.47	46.7	42.3	10.45	Night	12	All D
141	4.42	46.7	42.3	10.57	Day	3	D, D, C
142	3.90	35.3	31.4	9.06	Day	3	C, C, B
143	7.06	56.8	49.7	8.04	Day	3	All B
144	8.14	82.2	74.0	10.09	Day	3	C, C, D
145	2.98	31.4	28.4	10.53	Night	12	All D
151	6.56	65.1	58.5	9.93	Day	3	All D
152	7.53	72.4	64.8	9.61	Day	3	C, C, B
153	11.4	113	102	9.96	Day	3	B, C, C
154	8.15	85.6	77.5	10.51	Day	3	All D
155	2.48	18.6	16.2	7.50	Night	12	D, D, D, D, E, E, E, E, E, D, D, D
Overall Average	6.72	68.3	61.6	10.17		5.3	
Day Avg	7.53	76.6	69.1	10.18		3.3	
Night Avg	3.98	38.5	34.5	9.68		12.0	

When the model generated back-calculated emission rates are compared, it is interesting to see the emission rates differ by a factor of 10. Additionally, a comparison of the individual test data pieces reveal that the calculated emission concentrations from each model are extremely close.

Literature notes that assuming a continuously emitting source and homogenous turbulence, the Gaussian plume equation becomes a specific solution to the Lagrangian equation (Lamb and Seinfeld, 1973). A complete derivation of this solution can be found in the paper written by Lamb and Seinfeld (1973). However, in nonstationary and inhomogenous turbulence, the Gaussian equation estimates the Lagrangian model within a reasonable order of magnitude in practical circumstances (Lamb and Seinfeld, 1973). Thus, it is not all too surprising how close these emission rate back-calculations are. What is troubling, though, is the factor of 10 (an order of magnitude) difference between the two model calculations. This phenomena occurs in all of the trials, regardless of the atmospheric stability.

Additionally, it is interesting to note that the factor slightly decreases for test number 143, in which the stability class is B (moderately unstable) for each hour during the measurement time. In a moderately unstable atmosphere, the rate of cooling of an air parcel moving upward is less than that of the surrounding air, so it is rapidly accelerated upward due to buoyant forces (Cooper and Alley, 2002). Also, as the air parcel moves downward, buoyant forces cause the particle to accelerate downward due to the parcel warming at a slower rate than its surrounding environment (Cooper and Alley, 2002). Thus, this moderately unstable stability class is characterized by much more vertical mixing. This increased instability likely leads to an increase in the uncertainty in both model outputs and a decrease in the factor of difference between the models. This is because the Gaussian model does not model unstable atmosphere accurately (Trinity Consultants, 2000), and it serves as a solution to the Lagrangian model (Lamb and Seinfeld, 1973).

Conclusion

An evaluation of the emission rates generated by both the Industrial Source Complex (Gaussian) model and the WindTrax (backward-Lagrangian stochastic) model revealed that the calculated atmospheric concentrations (C_2 as used in equations 14 and 15) from each model using the average emission rate generated by the model are extremely close. Though, as previously mentioned and seen in Table 4, the average emission rates calculated by the models varied by a factor of 10. This is extremely troubling.

Current and future sources are regulated by the emission rate data from previous time periods. Emission factors are published for regulation of various sources, and these emission factors are derived based upon back-calculated model emission rates and site management practices. Thus, a factor of 10 ratio in the emission rates could prove troubling in terms of regulation if the model that the emission rate is back-calculated from is not used as the model to predict a future downwind pollutant concentration.

For example, it is necessary to look at interchanging the two back-calculated emission rates. If the emission rate generated by the ISC (Gaussian) model is used in the WindTrax (bLS) model and assuming the validity of the two models, then the predicted downwind concentrations will be almost a factor of 10 *less* than what the actual concentration is downwind of the source. An under-representation of the downwind pollutant concentration could lead to jeopardizing the public health and welfare, which is entirely opposite the mission of the Clean Air Act. Or the opposite situation could occur. If the emission rate generated by the WindTrax (bLS) model is used in the ISC (Gaussian) model and assuming the validity of the two models, the model would overpredict the downwind pollutant concentration, resulting in the over regulation of an emitting source. This affirms the thought that emission rates back-calculated from one model cannot be

used as the input into another model and result in valid downwind concentration predictions. Regulatory agencies are looking into moving to Calpuff as the dispersion modeling standard. Currently, there are a large number of published emission rates and emission factors used for regulatory compliance monitoring based off of the ISC model. Will these values be valid in other regulatory models? Future research needs to address this question.

Neither of these scenarios is desirable, but they illustrate the importance of properly reported data and the effect that improperly reported scientific data can have on the environment surround us. Nonetheless, realistic engineering and sound science is vital not only in the creation of public policy but also in the enforcement of this policy.

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