EVALUATION OF THE USE OF THE BOX MODEL TO DETERMINE EMISSION FLUXES FROM AREA SOURCES AND THE CORRESPONDING MODELED CONCENTRATIONS USING THE INDUSTRIAL SOURCE COMPLEX L. Barry Goodrich, Calvin B. Parnell, Jr., Ronald E. Lacey, Saqib Mukhtar, and Bryan W. Shaw Biological and Agricultural Engineering Department Texas A&M University College Station, TX

Abstract

Agriculture is currently facing more restrictive emission limits as a consequence of air quality regulations. A number of State Air Pollution Regulatory Agencies (SAPRAs) are focusing their efforts on particulate matter (PM) emissions from field operations. In particular, PM emissions from concentrated animal feeding operations (CAFO) are of concern. The problem with regulating air emissions from ground-level area sources (GLAS) is the lack of accurate emission flux data. This is partially due to the difficulties of directly measuring the emission rate of dust from a given source. In order to quantify the emissions from agricultural operations, net downwind concentrations are measured and the resulting concentrations are used to back into an emission flux using dispersion modeling. Emission fluxes can subsequently be reported as emission factors. One use of emission factors is for permitting new and existing sources. According to the EPA, "Modeling is the preferred method for determining emissions limitations for both new and existing sources," (EPA, 1999). It should be expected that emission factors will be used to estimate downwind concentrations using dispersion modeling and that the resulting estimated concentrations will be used in the air pollution regulatory process. The box model has been used in the past to estimate fluxes with the resulting fluxes being used in Industrial Source Complex–Short Term, Version 3 (ISC) to estimate downwind concentrations for estimating fluxes using the box model with the criterion that the subsequent concentrations with ISC will be conservative.

Introduction

It is important that the emission factors used in the air pollution regulatory process be accurate. Emission factors for groundlevel area sources (GLAS) are derived from emission fluxes. Emission fluxes are emission rates of pollutants in units of mass per unit area per unit time. Emission fluxes are used by state air pollution regulatory agencies (SAPRAs) to estimate downwind concentrations to compare to National Ambient Air Quality Standards (NAAQS) and for emission inventory purposes. If the emission factor is incorrect and too high, the resulting SAPRA actions can lead to costly and unnecessary installation of abatement measures. Conversely, if the emission factor is incorrect and too low, the resulting public exposure can pose a significant health risk. Since the NAAQS were designed to protect the public health (Cooper and Alley, 2000), it is vitally important that the predicted concentrations do not significantly under-estimate actual conditions. For these reasons it is important to develop a flux term from ambient concentration that will yield predicted concentrations in the same conditions that are greater than or equal to the sampled concentration when used as inputs in approved EPA dispersion models.

The goal of this study was to develop a process whereby the box model could be used to determine emission fluxes based upon measured concentrations and ISC could be used to predict downwind concentrations with the resulting fluxes. For the process to be acceptable, the predicted ISC concentrations were required to be larger than the measured concentrations used in the box model to determine the flux. The concept was a GLAS with concentration measurements being made at the edge of the GLAS. It was assumed that the emission flux would be uniform in the GLAS. The following data were used:

- the measured concentration was a constant 200µg/m³;
- the area source was a square with dimensions of 100m, 200m, and 500m on a side;
- the fixed box height was 4 meters;
- the sampler was located in the center of the area source 2 meters from the downwind edge and 1 meter high;
- the wind speed was a varied based on the stability class and assumed to come from an ideal direction.

The fluxes calculated with the box model were subsequently used as input for ISC to predict concentrations for the measured concentration location. The fluxes derived from use of the box model were considered to be conservative if the ISC results yielded concentrations higher than 200μ g/m³.

Box Model

The box model (Arya, 1999) in the context of GLAS emissions consists of a box placed over the source's surface to capture the emissions. The emissions are subsequently transported through the downwind end of the box. Concentration measurements are made on the upwind and downwind ends of the box. The net concentrations are assumed to represent the contribu-

tion made by the GLAS. (See figure 1.) Flocchini, et al. (2001) used a small scale modification of the box model to determine the flux of pollutants from an area source. Initially, Flocchini proposed a single box height of 4 meters with a uniform pollutant concentration on both the upwind and downwind ends of the box. The box was assumed to be the width of the downwind edge of the field. Mass balances were performed using average wind velocities, upwind and downwind box dimensions and measured concentrations. The average velocity (during the sampling period) multiplied times the downwind box end area yielded flow rate in units of volume per unit time. Flow rate multiplied by concentration yielded emission rate (mass per unit time). Emission rates divided by the area contributing emissions to the box (surface area) yielded flux. Equation 1 shows how the flux is calculated using this model.

$$Q_{A} = \frac{u \bullet Y \bullet H \bullet C \bullet \cos(\theta)}{X \bullet Y}$$
(1)

where

 Q_{A} = emission flux in micrograms per second per meter squared (µg-s⁻¹-m⁻²),

u = measured wind speed meters per second (m/s),

Y = width of field meters (m),

H = plume height (m),

C = net measured (downwind – upwind) concentration in micrograms per cubic meter ($\mu g/m^3$),

 θ = difference of the wind direction from ideal (0-45) (used as 0 for all tests), and

X = upwind length of field (m).

Note that equation can be simplified in that field width is both in the denominator and numerator. Flux is independent of field width (Y). It is assumed that the concentrations measured at the upwind and downwind ends of the box are uniform. Meister (2000) suggested that the vertical profile of pollutant downwind of an area source is better represented by a triangular distribution with a peak concentration occurring at approximately 25% of the total height of the plume and tapering down to zero at the top and bottom edge of the plume. Assuming the theoretical measured concentration is the maximum concentration a triangular distribution will yield a flux that is $\frac{1}{2}$ that of the uniform distribution. This is because the area of a triangle with the same base width (H) and peak concentration (C) as the uniform distribution has $\frac{1}{2}$ the area of the square. To be conservative, our approach was to assume a uniform distribution.

Industrial Source Complex

ISC is a steady state Gaussian plume model that can be used to predict downwind concentration from area sources (EPA, 1999). It calculates 1-hour average concentrations at receptor locations placed around the source. To determine the concentration at a receptor down wind of an area source ISC integrates the basic Gaussian equation over the area of the source as shown in equation 2 (EPA, 1995).

$$C = \frac{Q_A}{2\pi u_s} \int_X \frac{V}{\sigma_y \sigma_z} \left(\int_Y \exp\left[-0.5 \left(\frac{y}{\sigma_y} \right)^2 \right] dy \right) dx$$
(2)

where

C = concentration of pollutant (μ g/m³),

 $Q_{A} = \text{pollutant flux } (\mu g - s^{-1} - m^{-2}),$

V = vertical term used to describe vertical distribution of the plume,

 σ_{v} , σ_{z} = Pasquill-Gifford plume spread parameters based on stability class,

 $u_s =$ average wind speed at pollutant release height (m/s),

X = upwind direction, and

Y = cross wind direction.

ISC integrates the point source equation over the area of the source that is upwind of the receptor location. Therefore, receptors can be placed anywhere around or inside a source. The only limitation is the σ_z component goes to zero as the receptor distance approaches zero. This causes inconsistent results as the downwind distance (X) approaches 0. It is recommended that receptors not be placed less than 1 meter from any source. As the distance upwind of the sampler increases the vertical plume spread becomes very large. This large spread reduces the impact of that source location on the measured concentration.

In Gaussian modeling, it is assumed that the plume described by concentration versus distance from the source is normally distributed in the vertical and horizontal planes with standard deviations referred to as plume spread parameters (σ_y and σ_z). σ_y and σ_z are functions of the Pasquill-Gifford stability classes and downwind distances from the source. The use of the Gaussian model for elevated point sources assumes infinite dispersion of the plume in both directions as distance increases. The problem is that ground level area sources cannot have the plume extending below ground level. ISC corrects for this by reflecting the portion of the plume that is below ground level back above the ground. Therefore, ISC predicts the highest concentration at ground level (Meister, 2000).

Methods

For this analysis a constant wind direction was used for all tests. This removed the variation that arises with varying wind direction in ISC. All tests used a constant sampled concentration of $200\mu g/m^3$. This concentration was intended to represent a measured concentration of any pollutant down wind from an area source and was not meant to represent a specific type of pollutant. $200\mu g/m^3$ was used in the box model to determine an emission flux. The calculated flux was used with ISC to estimate downwind concentrations. This process was used for three, square fields; 100 m, 200 m and 500 m. The receptor location was the location used for the initial sampled concentration. The ISC predicted concentrations were compared to the sampled concentration of $200\mu g/m^3$. The calculation of emission flux using the box model used equation 1 which was simplified to equation 3.

$$Q_A = 800 \bullet \frac{u}{X} \tag{3}$$

where

 $Q_A = \text{emission flux } (\mu \text{g-s}^{-1} - \text{m}^{-2}),$ 800 = product of box height, cos(wind angle), and measured concentration (200 μ g/m³), u = wind speed), and X = field depth upwind of the sampler (100m, 200m, and 500m).

Results

Table 1 are the resulting fluxes calculated using the box model with a fixed measured concentration of 200 μ g/m³ and a downwind box height of 4 m. It is important to note that wind speed and flux are directly proportional and that flux and field size are inversely proportional. For example a doubling of the wind speed will double the calculated flux while a doubling of the field size will decrease the flux by ½. Due to the scalar nature of wind speed and emission flux in the box model, ISC will predict the same concentration for any wind speed and flux combination that is entered if all else is held constant (Table 2). This means that ISC is only dependent on the entered stability class and field size for the prediction of downwind concentration.

For the square field 100 meters on a side, ISC predicts a higher concentration than $200\mu g/m^3$ for all stability classes except A. As the field size increases, the predicted concentrations for all stability classes' decrease and the box model becomes less and less conservative (Table 3). The concentrations predicted are all 1-hour concentrations and do not reflect what would actually be modeled at that point for air pollution regulatory process. For example, for particulate matter the NAAQS are 24-hour average concentrations. To simulate 24-hour concentrations using dispersion modeling, 10 days of 1-hour meteorological data were used to calculate 24-hour concentrations using the meteorological data with associated stability classes at the 1-meter downwind receptor location (Table 4). The starting point was a measured concentration of 200 $\mu g/m^3$. The averaged estimated 24-hour concentrations for the 100m by 100m field was 472 $\mu g/m^3$; 200m by 200m field was 286 $\mu g/m^3$; and 500m by 500m field was 144 $\mu g/m^3$. The average 24-hour concentrations using the box model becomes less conservative.

The data shows that for a 100-meter by 100-meter filed the box model will provide a safety factor of approximately 2.4 (472/200). As the field becomes larger, the safety factor decrease and the box model process for estimating fluxes becomes less conservative. This can be explained by the fixed height of the box used in the box model. As the distance from the receptor to the emission point in the field becomes larger the plume spread increases to a point above the 4-meter height. One method used to compensate for the plume spread from emission points far from the sampler is to limit the "effective area" of the sampler to a 200-meter depth. For example, if sampling were conducted on a field that has a greater than 200 meters depth, the flux calculation from the box model would use 200 meters as X in equation 1. The calculated emission flux for the smaller effective area would apply to the entire field. The resulting flux would subsequently be used to determine the flux

and the actual field area would be used to determine downwind concentrations using ISC. The results from using this technique on a square 500-meter field are shown in Table 6.

Conclusions

The use of the box model with a fixed plume height of 4 meters for 1-meter downwind receptor location to determine flux for GLAS is a conservative provided the contributing depth of the field does not exceed 200 meters. By limiting the effective field depth of the GLAS to 200 meters or less the resulting flux used with the ISC modeled concentrations will always exceed the hourly measured concentrations. The over-prediction of the pollutant concentration by the ISC indicates that the use of the fixed height box model with the appropriate field depth limitations will yield a conservative estimate of the emission flux from GLAS.

References

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Table 1. Calculated emission fluxes (μ g-m⁻²-s⁻¹) using the box model for each field size and wind speed combination using a sampled concentration of 200 μ g/m³ and a box height of 4 meters.

Wind Speed	Depth of Field (X)			
(m /s)	100m	200m	500m	
1	8	4	1.6	
2	16	8	3.2	
3	24	12	4.8	
4	32	16	6.4	
5	40	20	8	
6	48	24	9.6	

Table	2	Industrial	Source	Complex		
predict	ted	downwind	concent	ration at a		
recepto	or l	ocated 1 m	eter fron	n the edge		
of a 100-meter by 100-meter field						

Wind Speed (m/s)	Emission Flux (µg/m²/s)	ISC Predicted Concentration (µg/m ³)
1	8	186
2	16	186
3	24	186
4	32	186
5	40	186
6	48	186

Table 3. Industrial Source Complex predicted down wind concentrations (μ g/m³) at a receptor that is 1 meter from the downwind edge of the field. The decreasing concentrations with increased field size represent less conservative estimates of flux from the box model.

Stability	Field Size						
Class	100m X 100m	200m X 200m	500m X 500m				
А	186	108	51				
В	238	140	68				
С	327	195	95				
D	478	288	145				
Е	587	360	185				
F	856	529	275				
Average	445	270	137				

Table 4. Hourly stability class frequency for 10 days as determined from measured meteorological data in College Station, TX (Fritz, 2002) and the corresponding 24-hour average predicted concentrations (μ g/m³) for three field sizes using ISC.

	S	Sta	bili	ity (Class	5		Field Size	
	Α	B	С	D	Е	F	100m X 100m	200M X 200m	500m X 500m
Day 1	2	4	0	11	6	1	457	276	140
Day 2	0	0	7	13	4	0	452	273	137
Day 3	0	0	0	21	2	1	503	304	154
Day 4	0	3	6	9	5	1	449	271	137
Day 5	0	5	2	9	7	1	463	280	142
Day 6	0	0	3	11	10	0	505	306	155
Day 7	0	0	1	18	5	0	494	299	151
Day 8	0	0	1	14	9	0	513	311	158
Day 9	0	6	3	11	4	0	417	251	126
Day 10	0	2	5	7	10	0	472	286	145
Avera	ge	Co	nce	ntra	tion		472	286	144

Table 5. Predicted downwind ISC 1-hour concentrations ($\mu g/m^3$) for a 1000-meter by 1000 meter field with an emission flux calculated using the box model with an effective field area of 200 meters by 200 meters.

Stability Class	1-Hour Concentration
А	126.7
В	169.6
С	237.2
D	362.5
E	463.3
F	687.4

Table 6. 24-hour predicted concentrations (μ g/m³) with Industrial Source Complex for 10 days of real-world meteorological data (with associated stability classes) measured in College Station, TX (Fritz, 2002) for a 1000-meter, square field using emission fluxes calculated using the box model with effective field depth of 200 meters.

Day	24-Hour Concentration
1	349
2	343
3	384
4	342
5	355
6	389
7	378
8	395
9	315
10	362



Figure 1. Schematic diagram of a GLAS of pollutants as conceived in the box model. The emission fluxes are assumed to be uniform and constant over the GLAS surface. The concentrations measured at both the upwind and downwind ends are assumed to be constant $(200 \ \mu g/m^3)$ with a box height equal to 4 m.