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Sensors and Actuators B 106 (2005) 122–127
SENSORS AND ACTUATORS B CHEMICAL
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Eulerian-Lagrangian model for predicting odor dispersion using instrumental and human measurements

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Available online 2 September 2004

Abstract

A Eulerian-Lagrangian model was used to predict the trajectory and spatial distribution of odor and odorants downwind from an industrial facility with multiple sources of odor emissions. Specifically, the model was used to simulate the dispersion of odor from a confined animal feeding operation (CAFO) under different meteorological conditions: (1) during daytime when the boundary layer is usually turbulent due to ground-level heating from solar short wave radiation, and (2) during the evening when deep surface cooling through long-wave radiation to space recreates a stable (nocturnal) boundary layer. Aerial photographs were taken of the CAFO, and the geographical area containing the odorant sources was partitioned into 10 m^2 grids. Relative odorant concentrations present at each grid point that corresponded to an odor source were measured on site and then entered into a database. The predicted odor dispersion distance was found to be greater at night-time than during daytime and was consistent with field reports from individuals living near the CAFO. The model utilizes single numbers that represent relative concentrations or intensities (e.g. from an electronic nose or human judgments) to simulate downwind dispersion. The advantages of this algorithm over standard Gaussian plume models are that: the velocity variances and covariances among its three components, integral time scale (a measure of eddy coherency), and complex boundary conditions (e.g. complex release points, surface boundary conditions) are explicitly considered.

Keywords: Odor dispersion; Odorant concentration; Odor intensity; Prediction of odor downwind

1. Introduction

Long distance dispersion of odor is a problem in communities surrounding many odorous industries such as confined animal feeding operations (CAFOs), wastewater treatment plants, composting facilities, and paper mills. This paper describes a paradigm for predicting the trajectory of odorous emissions from a CAFO with multiple sources of odor. Measurements from machines or humans can be used as input to predict the long-range transport and deposition of odorants (compounds that produce odor sensations) and odor (the sensation).

2. The dispersion model

The mechanistic model underlying the odor projections in this paper has been used previously to predict the long-distance dispersal of seeds by wind [1]. It is based on stochastic differential equations for turbulent diffusion that utilize a Eulerian-Lagrangian approach [2,3]. The approach solves for the flow statistics in the Eulerian frame of reference and then proceeds to solve for air parcel trajectories in the Lagrangian frame of reference. The Eulerian frame of reference models the flow statistics (i.e. velocities) at a fixed point, while the Lagrangian trajectory calculations follow the coordinates of an individual air parcel until this air parcel intercepts the ground surface or escapes from the atmospheric boundary layer (see [4]).

Overall, the model uses the spatial distribution of odor concentrations at emission sources (in steady-state conditions) to predict the spatial distribution of odor and odorants downwind. The model can predict transport over the terrain under a variety of planetary boundary layer (PBL) conditions including the variations over the diurnal cycle. The PBL is the part of the atmosphere closest to the ground (i.e. where we live); it varies in thickness between 100 m at night to 3 km during daytime. In daytime conditions, the boundary layer is usually very turbulent due to ground-level heating resulting

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doi:10.1016/j.snb.2004.05.067

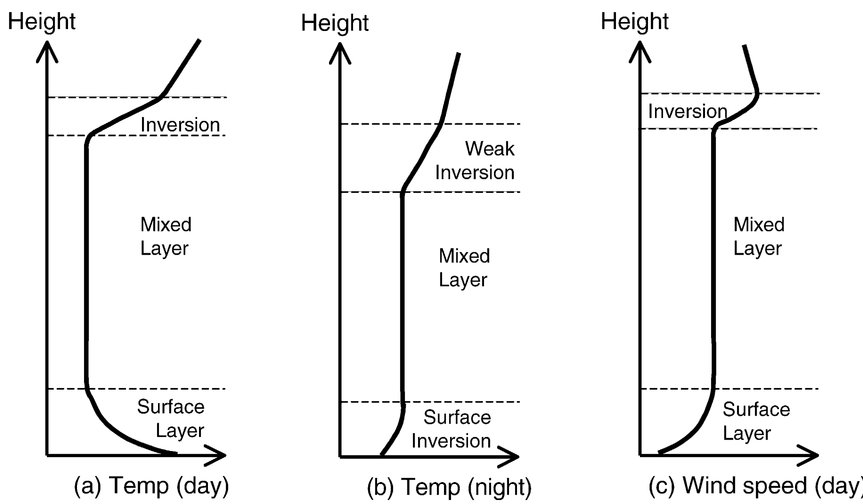


Fig. 1. (a) and (b) Height and temperature conditions of the boundary layer during the day and night, respectively; (c) logarithmic relationship of height and wind speed in the surface layer.

from solar short-wave radiation [5]; dispersion results from turbulent mixing in both vertical and horizontal directions. In the evening, deep surface cooling through long-wave radiation to space recreates a stable nocturnal boundary layer of statically stable air with weaker, sporadic turbulence, above which is a residual layer (basically the leftover part of the daytime mixed layer; see Fig. 1a and b). Because vertical motion and turbulence is suppressed at night, odorants are not carried upward as readily as during the daytime, and mixing is weak. Consequently, odorants (such as those emanating from flowers and malodorous sources) smell much stronger on summer nights than during the day because of the stillness of the air. The model utilizes the observed mean velocity near the surface and extrapolates this velocity at all heights using the analytic function in Fig. 1c.

3. Applying the model

The specific example used in this paper illustrates the fate and transport of odor emitted from a swine operation with multiple odor sources including an effluent lagoon, housing units, and land application of effluent from the lagoons onto agricultural fields by a spraying process. Aerial photographs were taken of the farm (see Fig. 2), and the geographical area containing the odorant sources was partitioned into $10\,m^2$ grids. Relative odorant concentrations present at each grid point that corresponded to an odor source (see Fig. 3) were determined from on site measurements and then entered into a database. The computer code for the model was employed to predict the odor downwind for a given set of meteorological conditions. In the example here, human odor measurements were the basis of the modeling. The total intensity response from an electronic nose or a portable photo-ionization detector (PID) can also be used to determine the intensity of odorant sources. However when using a device, the relationship between the machine and human odor intensity must be established.

In order to perform the dispersion modeling for odor, it is necessary to determine a mathematical relationship between odor perception and measurable concentration of odorants. That is, the psychophysical relationship between psychological or sensory qualities on the one hand must be related to physical or stimulus quantities on the other. This is necessary because it is the odorants (physical entity) and not the odor (sensory property) that is dispersed. An overview of the literature on the senses indicates that perceived intensity tends to be exponentially related to stimulus magnitude [6]. In sensory systems other than chemical senses of smell and taste, the continua on which sensations vary (i.e. wavelength, frequency) are known. In audition, for example, the relationship between intensity and the physical signal is logarithmic, and the standardized universal constant is the decibel. That is, the sensation perceived by a human is related logarithmically to the energy transmitted to the auditory receptors. Furthermore, the decibel is unrelated to the source or quality of the sound. In olfaction, on the other hand, the sensation is more complex because it depends both on the concentration of the stimulus and on its chemical composition.

Odorous emissions consist of mixtures of many molecules that in aggregation induce a unique intensity and quality. That is, the types of compounds in the airborne mixture and their relative concentrations both affect the perceived odor intensity [7].

4. Simulated results and discussion

A hypothetical example of the relationships between three individual odorants and perceived intensity is given in Table 1. For Odorant A, many molecules are necessary to induce a strong odor, while relatively fewer molecules

Fig. 2. Aerial view of a swine facility illustrating housing units and lagoon.

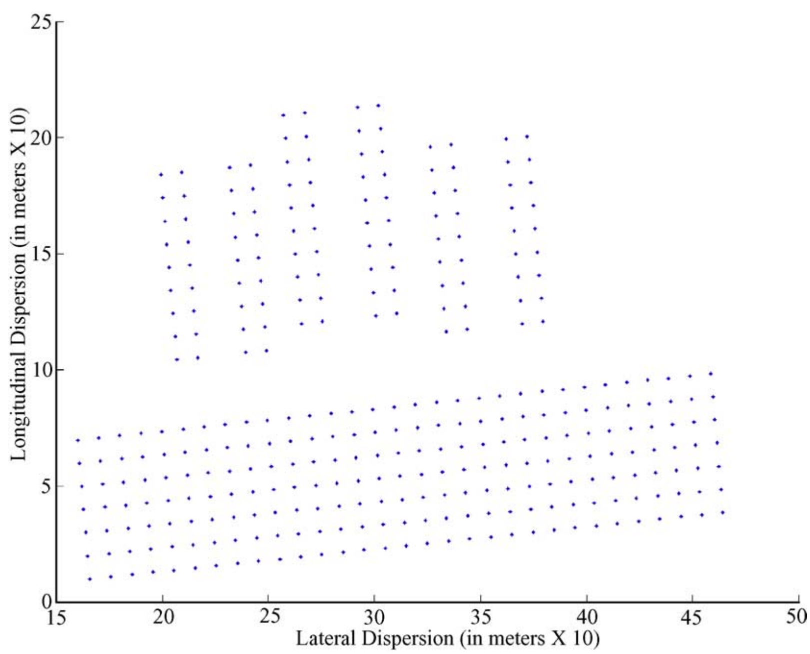


Fig. 3. Sources of odor at each grid point; measured relative intensity is entered into database.

are necessary to produce the same strong odor intensity in Odorants B and C. The logarithmic relationship between perceived odor intensity and number of molecules is shown in Fig. 4. The intensity of a mixture of these compounds, however, cannot be easily predicted from the raw concentration values. Even if the actual ratios of these compounds in a mixture were known, it still would not be possible to predict the resulting odor intensity of the mixture due to the unknown nature of interaction of the mixture with the nasal receptors.

The relationship between perceived odor intensity and number of molecules in ambient air on a swine facility are even less predictable due to the presence of hundreds of different types of molecules. Thus, the model utilizes hy-

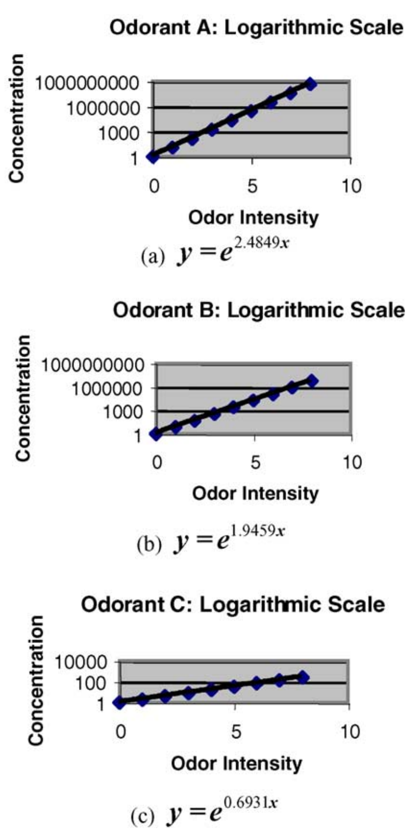
Table 1
Relationships between three hypothetical odorants and perceived odor intensity

Odor intensity	A: concentration (ppt)	B: concentration (ppt)	C: concentration (ppt)
0 = None at all	1	1	1
1 = Very weak	12	7	2
2 = Weak	144	49	4
3 = Moderately weak	1728	343	8
4 = Moderate	20,736	2401	16
5 = Moderately strong	248,832	16,807	32
6 = Strong	2,985,984	117,649	64
7 = Very strong	35,831,808	823,543	128
8 = Maximal	429,981,696	5,764,801	256

pothetical “odorous air parcels” to predict odor downwind using an equation that can be confirmed by experimental odor intensity measurements. Odorous air parcels are used for modeling rather than the sensations themselves because it is the physical odorants that are dispersed. For the example illustrated in this paper, we developed an equation to represent the relationship between perceived odor intensity determined in the field by a trained odor panel and “odorous air parcels” released by the mathematical model at each 10 m^2 grid that decay over distance:

$$y = 33.546\,e^{x}$$

where x is the odor intensity on a scale from 0 to 8 (0 = none at all; 1 = very weak; 2 = weak; 3 = moderately weak; 4 = moderate; 5 = moderately strong; 6 = strong; 7 = very strong; and 8 = maximal) and y is the number of “air parcels” released. When odor is maximal (e.g. rated 8) at a specific 10 m^2 grid, the number of odorous air parcels released will be 100,000. When odor is rated moderate (e.g. rated 4), only 4978 odorous air parcels will be released. When no odor is perceived at a specific 10 m^2 grid (e.g. rated 0), no odorous air parcels will be released from the 10 m^2 grid. Thus, the model described above predicts the exponential decay over distance when odorous air parcels that are related monotonically to human odor intensity are released from a grid of sources arranged to mimic the emissions from an odorous facility. The model is then confirmed by experimental measurements.



(a) $y = e^{2.4849x}$

(b) $y = e^{1.9459x}$

(c) $y = e^{0.6931x}$

Fig. 4. Relationships between odor intensity and concentration for three hypothetical odorants.

The dispersion plots in Fig. 5 illustrate the predicted odor intensity for the swine operation shown above during the day and at night. The plots utilize the logarithmic values of the number of odorous air parcels. That is, the number of odorous air parcels that reach any grid location downwind on dispersion were plotted because odor intensity (as noted above) is exponentially related to odorant concentration.

The findings here demonstrate odor dispersion prediction under different meteorological conditions, e.g. dispersion at night-time is greater than during daytime. This finding coincides with field reports from individuals living near CAFOs. The advantages of this algorithm over standard Gaussian plume models are that: the velocity variances, integral time scale (a measure of eddy coherency), and complex boundary conditions (e.g. complex release points, surface boundary conditions) are explicitly considered. All that is needed for input to the model are single numbers that represent relative concentrations or intensities of the various odor sources. These numbers can be determined using the total response of all sensors of an E-nose, a photoionization detector (PID), or human odor intensities. However, if an electronic nose or PID is used for the modeling, a mathematical relationship between the machine output and human sensory perception is required. This is because the perceived intensity depends on the specific chemical compounds that constitute the odor.

5. Other applications of the model

An important practical application of the modeling procedure described here is the prediction of the potential ef-

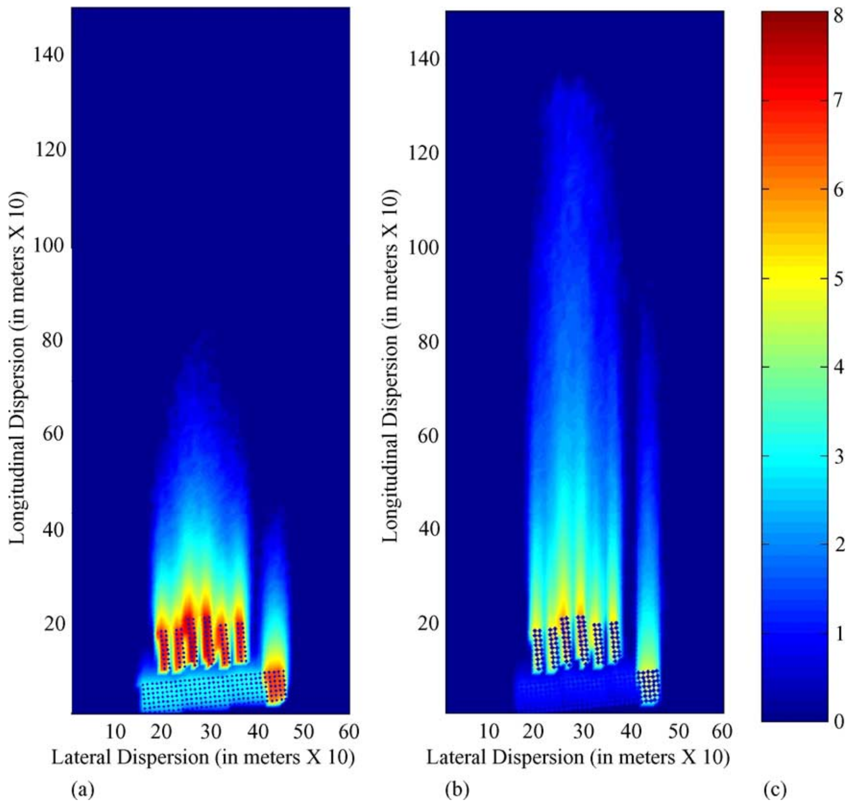


Fig. 5. Predicted dispersion of odorous air parcels during (a) daytime and (b) night-time for the same reference wind speed at 10 m height. The intensity scale is displayed in (c).

fectiveness of odor control technologies alone and in aggregate for reducing odor downwind of odorous industrial facilities. Typical examples of processing procedures to reduce odor at the source are wet scrubbers, activated carbon adsorbers, thermal oxidation, biofilters, and bioscrubbers. These procedures can be costly to install so it is necessary to predict a priori which intervention (or combination) will be most effective. In wet scrubber reactors, odorous air contacts a chemical solution (usually containing sodium hypochlorite and caustic soda) that allows absorption and subsequent oxidation of odorous compounds such as H_2S. Activated carbon adsorbers utilize caustic-impregnated carbon to remove H_2S and a virgin-activated carbon to remove VOCs and non-H_2S odorants. Thermal oxidation heats odorous air to high temperatures that oxidize the odorous compounds. Biofilters remove odorants by transporting the odorous emissions through porous natural media such as compost, soil, wood chips, or peat. Bioscrubbers oxidize odorous compounds as air is passed through a biologically active medium (e.g. bacteria adsorbed into a liquid film).

6. Conclusions

The potential effectiveness for various arrangements and types of odor remediation methodologies at an odorous facility in neighboring communities can be modeled using the method described above before expensive construction commences. Dispersion modeling utilizing single numbers that represent relative concentrations or intensities (e.g. from an E-nose or human judgments) of the current odor sources for a facility can be compared with dispersion modeling of expected relative concentrations after installation of odor remediation equipment. This will optimize the choice of appropriate odor control technologies for a given industrial operation.

Acknowledgements

The model development was supported, in part, by the National Science Foundation (NSF-EAR and NSF-DMS), the Department of Energy through the National Institute for Global Environmental Change (NIGEC) and Terrestrial Carbon Processes (TCP) programs.

References

[1] R. Nathan, G.G. Katul, H.S. Horn, S.M. Thomas, R. Oren, R. Avissar, S.W. Pacala, S.A. Levin, Mechanisms of long-distance dispersal of seeds by wind, Nature 418 (6896) (2002) 409–413.

[2] C.I. Hsieh, G.G. Katul, J. Schieldge, J.T. Sigmon, K.K. Knoerr, The Lagrangian stochastic model for fetch and latent heat flux estimation above uniform and nonuniform terrain, Water Resour. Res. 33 (3) (1997) 427–438.

[3] G.G. Katul, J.D. Albertson, An investigation of higher-order closure models for a forested canopy, Bound. Lay. Meteorol. 89 (1) (1998) 47–74.
[4] H.C. Rodean, Stochastic Lagrangian models of turbulent diffusion, Meteorol. Monographs 26 (48) (1996).
[5] R.B. Stull, An Introduction to Boundary Layer Meteorology, Kluwer Academic, Dordrecht, 1988, p. 666.
[6] L.E. Marks, Sensory Processes. The New Psychophysics, Academic Press, New York, 1974.
[7] S.S. Schiffman, J.L. Bennett, J.H. Raymer, Quantification of odors and odorants from swine operations in North Carolina, Agr. Forest Meteorol. 108 (3) (2001) 213–240.

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