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ANALYSIS OF ENSEMBLE AVERAGED CONCENTRATIONS AND FLUXES IN A TRACER PUFF

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ABSTRACT

This research was initiated to analyze tracer concentrations and fluxes in a diffusing puff released from an instantaneous ground level point source. The concentration data used was made available by the Battelle Memorial Institute. Three basic steps are performed. First, an estimate of the ensemble averaged tracer fluxes is developed. Secondly, an estimate of the ensemble averaged tracer concentration is obtained. Then the estimates are used to determine concentrations and fluxes which satisfy the diffusion equation and are as close to the estimates as possible.

The tracer fluxes are estimated as the negative of the products of the appropriate diffusivities and concentration gradients. The diffusivities are derived using the fact that they are proportional to a characteristic length and velocity scale. This approach yields diffusivities which are the diffusion rates for a Gaussian puff. The flux estimates are shown to satisfy the diffusion equation for all puff diffusion rates when combined with a Gaussian concentration model.

Since the available observations are too sparse to use alone in obtaining a concentration analysis in space and time, a concentration model is developed to provide data at grid points where there are no observations. This model is a modification of the Gaussian one, taking into account surface scavenging and wind shear. A variational technique then incorporates the observations and model data into concentration analyses. A variable observational weight forces the analyses towards the observations, and time filtering in a Lagrangian coordinate system allows the effect of an observation to be felt over several analysis times. Spatial filtering spreads the effect of the observations and helps eliminate short waves. The resulting analyses conform to the observations and provide reasonable concentration distributions in both space and time.

A model to estimate the ensemble averaged concentration is developed based upon the above analyses. Due to the random nature of turbulence, concentrations averaged over many trials should be more nearly normally distributed in the horizontal than the analyses are. Therefore, the model estimates are normally distributed in the horizontal, but the centroid of the horizontal distribution at a given level is displaced downwind relative to the centroid at the adjacent lower level. This type

of distribution is in general agreement with the concentration analyses described above. The ensemble averaged concentration estimates are then made to conform to the analyses as closely as possible using a least squares technique. Concentration gradients are obtained from these estimates for use in computing the estimated fluxes.

The concentration and flux estimates are combined with the diffusion equation in a variational functional. The Euler equations resulting from taking the first variation of the functional may be solved so that concentrations and fluxes obtained satisfy the diffusion equation and are as close to the estimates as the observational weights allow. It is assumed that these quantities are the ensemble averaged concentrations and fluxes.

The ensemble averaged concentrations are close to the analyses obtained from the first variational technique in magnitude, but the ensemble averaged horizontal distributions are more Gaussian. Furthermore the ensemble averaged concentrations are in very close agreement with the observed concentrations. Since they also satisfy the diffusion equation, the ensemble averaged concentrations obtained are very reasonable.

The ensemble averaged concentrations and horizontal fluxes are very close to their estimates, but the vertical flux differs significantly from its estimate. Due to the manner in which the observational weights were chosen, this indicates that the concentration and horizontal fluxes may be modeled in the manner in which the estimates are obtained, but some modification must be made to correctly model the vertical flux. Since the horizontal fluxes are close to their estimates, they are nearly proportional to the concentration gradients. Therefore, in this case, the diffusivity concept has a physical significance. Since the diffusivities are the diffusion rates of the puff, they can be measured in the atmospheric surface layer.

ABBREVIATIONS AND SYMBOLS

A	scavenging factor
$\bar{A}$	amplitude of filtered analysis
$\tilde{A}$	amplitude of observations
a_1	constant of proportionality for downwind standard deviation relation
a_2	constant of proportionality for crosswind standard deviation relation
a_3	constant of proportionality for vertical standard deviation relation
B	the value of $\hat{\chi}$ on the ordinate
b_1	time power for downwind standard deviation relation
b_2	time power for crosswind standard deviation relation
b_3	time power for vertical standard deviation relation
$C(\tau)$	correlation between $u'(t_f - \tau)$ and $u'(t_f)$
$C(t)$	dimensionless time dependent parameter
C_1	time dependent proportionality parameter
C_2	correlation between ℓ_x and u'
C_3	ratio of C_1 to C_2
F	over relaxation factor
F_x	flux in the x direction
F_y	flux in the y direction
F_z	flux in the z direction
$\hat{F}_x$	estimated flux in the x direction

$\hat{F}_y$ estimated flux in the y direction

$\hat{F}_z$ estimated flux in the z direction

G constant determined by interval-halving

K_x diffusivity in the x direction

K_y diffusivity in the y direction

K_z diffusivity in the z direction

k wave number

L_x wavelength, downwind direction

$L_{y \text{ or } z}$ transverse wavelength

ℓ_c characteristic length scale

ℓ_x distance that a tracer particle is displaced from the puff centroid in the x direction

Q Actual source strength

Q' virtual source strength

R response function

R^ν residual of the Euler equation at the ν-th iteration

r detector count rate

T Lagrangian integral scale

T_o period of the wave

t travel time from the source

t_i lower limit of the time integration

t_f observation time

Δt time interval

$\bar{u}$ mean wind velocity

u' turbulent wind fluctuation in the x direction

u_o effective transport wind speed

v' turbulent wind fluctuation in the y direction

VR variance of the residual of the diffusion equation

w' turbulent wind fluctuation in the z direction

x distance of the puff centroid from the source

x' distance that a tracer particle is carried in the x direction by turbulent wind fluctuations

y crosswind distance from the puff centroid

y' distance that a tracer particle is carried in the y direction by turbulent wind fluctuations

Δx downwind grid interval

Δy crosswind grid interval

z vertical distance from the puff centroid

z' distance that a tracer particle is carried in the z direction by turbulent wind fluctuations

Δz vertical grid interval

z_o height at which u_o is determined

α_1 observational weight

$\alpha_2, \alpha_3, \alpha_4, \alpha_5$ filtering weights

β $-d\ln A/dt$

$\gamma_1, \gamma_2, \gamma_3, \gamma_4$ observational weights

λ_m spectral scale of the vertical component of motion

ε rate of dissipation of turbulent kinetic energy per unit mass of air

σ_x concentration standard deviation in the x direction

σ_y concentration standard deviation in the y direction

σ_z concentration standard deviation in the z direction

τ $t_f - t$

φ	azimuthal angle to puff centroid
χ	ensemble averaged puff concentration
$\hat{\chi}$	krypton-85 concentration
$\bar{\chi}$	analyzed concentration
$\tilde{\chi}$	model concentration or, if available, krypton-85 concentration
$\langle\chi\rangle$	ensemble averaged concentration estimates

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CONTENTS

Abstract iii
Figures. vi
Tables viii
Abbreviations and Symbols. ix
Acknowledgment xiii

1. Introduction 1
2. Review of Pertinent Diffusion Theories and Assumed Puff Distribution. 3
   The Gaussian model. 3
   Diffusivity and the diffusion equation. 4
   The gradient transfer hypothesis. 5
   The statistical theory of dispersion. 6
3. Determination of the Turbulent Flux Estimates. . . . 10
   Diffusivity and the diffusion rate. 10
   Satisfaction of the diffusion equation. 11
   Boundary conditions 11
   A relationship with the statistical theory of turbulence 12
   Expressions for the fluxes. 15
4. Data Utilized in This Research 16
   Krypton-85 as an atmospheric tracer 16
   Puff dimensions 20
5. Determination of the Ensemble Averaged Concentration Estimate. 25
   The initial concentration model 25
   Combining the model data and observations . . . 36
   Filtering characteristics 39
   Boundaries. 45
   Analyzed concentrations 45
   Concentration estimates 61
6. Combining Flux and Concentration Estimates 64
   The variational formalism 64
   Analysis of a Gaussian puff 66
   Analysis of puffs P5 and P7 70
   Ensemble average concentrations 76
7. Conclusions. 81

Bibliography 84
Appendices

A. Derivation of the expression for diffusivity 87
B. Centered finite difference algorithms. 90
C. Numerical solution of the analysis functional. . . . 92
D. Numerical solution of the functional combining flux and concentration estimates 94

FIGURES

Number		Page
1.	Tentative profiles of vertical diffusivity.	7
2.	Motion of a tracer particle in a turbulent flow . . .	7
3.	Motion of two particles in a puff	13
4.	Relationship between ℓ_x and u'.	13
5.	Schematic representation of the field grid.	17
6.	Concentrations at the 1.5 m level for test P5	30
7.	Concentration profiles on the 114° azimuth for test P5	31
8.	Concentrations at the 1.5 m level for test P7	32
9.	Concentration profiles on the 114° azimuth for test P7	33
10.	Relationship between observation and model coordinates	34
11.	Time cross section at grid point 13,8,3 for test P5 .	34
12.	Time cross section at grid point 16,7,5 for test P5 .	37
13.	Response function using $\alpha_2/\alpha_1 = 20$, $\alpha_3/\alpha_1 = 2.5$ and $\alpha_4/\alpha_1 = 50$.	41
14.	Response function using $\alpha_2/\alpha_1 = 1$, $\alpha_3/\alpha_1 = .125$ and $\alpha_4/\alpha_1 = 2.5$	43
15.	Analyzed concentrations at the 1.5 m level for puff P5	48
16.	Analyzed concentrations at the 6.1 m level for puff P5	52
17.	Analyzed concentrations at the 1.5 m level for puff P7	55

18. Analyzed concentrations at the 6.1 m level for puff P7 58

19. Ensemble averaged concentration for Case 1, test P5, at the 1.5 m level. 67

20. Ensemble averaged downwind flux for Case 1, test P5, at the 1.5 m level. 67

21. Ensemble averaged crosswind flux for Case 1, test P5, at the 1.5 m level 68

22. Ensemble averaged vertical flux for Case 1, test P5, at the 1.5 m level 68

23. Ensemble averaged concentration profile for Case 1, test P5 69

24. Ensemble averaged concentration for Case 2, test P5, at the 1.5 m level 69

25. Ensemble averaged downwind flux for Case 2, test P5, at the 1.5 m level 73

26. Ensemble averaged crosswind flux for Case 2, test P5, at the 1.5 m level 73

27. Ensemble averaged vertical flux for Case 2, test P5, at the 1.5 m level 75

28. Ensemble averaged concentration for Case 2, test P7, at the 1.5 m level 75

29. Ensemble averaged downwind flux for Case 2, test P7, at the 1.5 m level 77

30. Ensemble averaged crosswind flux for Case 2, test P7, at the 1.5 m level 77

31. Ensemble averaged vertical flux for Case 2, test P7, at the 1.5 m level 78

32. Ensemble averaged concentration profile for Case 2, test P5 78

33. Ensemble averaged concentration profile for Case 2, test P7 79

TABLES

Number Page

1. Meteorological Data for the Two Tests 18

2. Measurements of Puff Dimensions 21

3. Puff Diffusion Rates. 23

4. Available Data for Test P5 When the Puff Centroid is Near the 200 m Measuring Arc. 26

5. Available Data for Test P7 When the Puff Centroid is Near the 200 m Measuring Arc. 27

6. Parameters Optimized to Fit the Model to Observations. 29

7. Analyzed Concentrations for Test P5 When the Puff Centroid is Near the 200 m Measuring Arc. 46

8. Analyzed Concentrations for Test P7 When the Puff Centroid is Near the 200 m Measuring Arc. 47

9. Parameters Optimized to Fit an Ensemble Averaged Estimate to the Analysis. 62

10. Diffusivities and Their Variances 71

11. Correlation Between Fluxes. 72

SECTION 1

INTRODUCTION

This paper describes an analysis technique which has been developed to analyze ensemble averaged concentrations and fluxes for tracer puffs diffusing in the surface layer. It is not possible to achieve this goal using available observations directly, because it is impossible to measure the ensemble averaged properties of the puffs. The ensemble average is an average taken over a large number of individual events which occur under identical ambient conditions.

It is sometimes possible to estimate ensemble averages from time averages. As shown by Wyngaard (1973), the turbulent properties of a stationary flow may be derived from time averages, if the averaging period is sufficiently long. However, a tracer puff residing in stationary flow is continuously changing, due to the diffusion process. The puff, unlike a tracer plume, can never achieve a steady state. Therefore, long time averages are not representative of the ensemble averaged properties of the puff and other means of obtaining the concentrations and fluxes must be developed.

Fluxes are derived which satisfy the diffusion equation for a Gaussian puff spreading out at an arbitrary rate. These fluxes are then used as estimates of the ensemble averaged fluxes for a puff diffusing in the surface layer.

Concentration estimates may be based upon observed data; however, this information is usually too sparce to use alone in analyzing concentrations. Therefore, analyses are obtained by combining the data with a concentration model using a variational technique. The model is a modification of the Gaussian distribution which accounts for wind shear and surface scavenging. The ensemble averaged concentration is more nearly normally distributed than is the concentration in an individual puff, so the ensemble averaged concentration estimates are produced by the model such that they are normally distributed in the horizontal and as close to the analyses as possible.

In the next step the flux and concentration estimates are combined to produce ensemble averages which satisfy the diffusion equation. This is accomplished through the use of a variational formalism, which forces satisfaction of the diffusion equation