PNL-SA-7587

CONF-790721--3

LAGRANGIAN SIMILARITY MODELING OF VERTICAL DIFFUSION FROM A GROUND-LEVEL SOURCE

MASTER

T. W. Horst

To be presented at the Second Symposium on Turbulent Shear Flows - July 2-4, 1979. Imperial College, London, England.

Prepared for
the U.S. Department of Energy
under Contract EY-76-C-06-1830

Pacific Northwest Laboratory
Atmospheric Sciences Department
Richland, Washington 99352

DISCLAIMER

LAGRANGIAN SIMILARITY MODELING OF VERTICAL DIFFUSION FROM A GROUND-LEVEL SOURCE

Thomas W. Horst

Abstract: Several alternate Lagrangian similarity predictions of turbulent diffusion in a thermally-stratified turbulent shear flow were compared with the Prairie Grass ground-level, crosswind-integrated tracer concentration data. The best agreement with the data was found by assuming that the eddy diffusivity K of a passive contaminant corresponds to that of heat, by using an exponent r equal to 1.5 or 2 in the vertical contaminant distribution $\exp[-(\bar{z}/b\bar{z})^r]$, and by using Chaudhry and Meroney's equation

$$d\bar{z}/dx = K(\bar{z})/\bar{z}u(c\bar{z})$$

for the downwind growth of the mean height $\bar{z}$ of the diffusing contaminant.

Nomenclature

b	constant of vertical distribution
c	constant relating advection wind to $\bar{z}$
c_p	specific heat of air at constant pressure
f	dimensionless wind profile, Eq. (11)
g	acceleration due to gravity
H	vertical heat flux
K	eddy diffusivity of contaminant
K_h	eddy diffusivity of heat
K_m	eddy diffusivity of momentum
k	von Kármán's constant
L	Obukhov length $[-u_*{}^3\rho c_p\theta/(kgH)]$
Q	release rate of contaminant
Ri	Richardson number $[g(\partial\theta/\partial z)/\theta(\partial u/\partial z)^2]$
p	constant = 1.55, Eq. (15)
r	exponent of vertical distribution
u	mean wind speed
u_*	friction velocity $[(\tau/\rho)^{\frac{1}{2}}]$
x	downwind coordinate
$\bar{x}$	mean downwind distance of contaminant
z	vertical coordinate
$\bar{z}$	mean height of contaminant
z_o	roughness length
α	K_h/K_m or ϕ_m/ϕ_h at neutral stability
Γ	gamma function, $\Gamma(z) = \int_0^\infty t^{z-1}e^{-t}dt$
θ	potential temperature
ρ	density of air
τ	surface shearing stress
ϕ_h	dimensionless temperature gradient $[u_*kz(\rho c_p/H)\partial\theta/\partial z]$
ϕ_m	dimensionless wind shear $[(kz/u_*)\partial u/\partial z]$
χ	crosswind-integrated contaminant concentration

1. Introduction

Lagrangian similarity theory is a promising basis for the description of vertical diffusion from a ground-level source in a thermally-stratified boundary layer. The dimensional relationships of Monin (1) and Batchelor (2) have been quantified by comparing Lagrangian similarity to gradient-transfer theory (3, 4, 5, 6). However, application of similarity theory to the prediction of contaminant concentrations also depends on knowing: the proper eddy diffusivity for passive contaminants; and the form of the vertical distribution of contamination and how it depends on thermal stability.

This paper investigates these points by comparing alternative Lagrangian similarity predictions to atmospheric measurements of the ground-level, crosswind-integrated concentrations (CWIC) of a diffusing tracer, rather than to direct measurements of the vertical spread of the tracer. This approach has the disadvantage that additional assumptions are required to specify the vertical contaminant distribution, but it also has several advantages. Ground-level tracer measurements are made more often than elevated measurements, simply because ground-level measurements are more economical, and the measurement arrays generally have larger numbers of samplers. Thus more ground-level measurements are available at large extremes of thermal stability and at large downwind distances. Second, the ground-level CWIC estimates are potentially more reliable since a larger number of concentration samples contribute to a single estimate of the CWIC than is generally the case for direct estimates of the vertical spread and also since the crosswind edges of the tracer plume are more likely to be well-defined than the upper edge.

2. Prediction of the Ground-Level Concentration

Monin-Obukhov similarity theory proposes that the properties of turbulence within a thermally-stratified surface flux layer are determined solely by z, τ, H, ρ, c_p and g/θ. Equivalently, these may be reduced to the height z, the friction velocity u_*, and the Obukhov length L. Lagrangian similarity theory (7) extends this proposal to the diffusion of passive contaminants within the surface flux layer. The mean rate of vertical displacement for particles released from ground level is assumed to be

$$\frac{d\bar{z}}{dt} = au_{*}G(\bar{z}/L) \quad , \tag{1}$$

where $\bar{z}$ is the mean height of the diffusing material and G is a function of thermal stability equal to unity for adiabatic conditions. The mean rate of horizontal displacement is assumed to be

$$\frac{d\bar{x}}{dt} = u(c\bar{z}) \quad . \tag{2}$$

Given the constants a and c and functional forms for G and the wind profile, $\bar{z}$ may then be determined as a function of $\bar{x}$, u_* and L.

Assuming that vertical diffusion from a ground-level source can also be described by gradient-transfer theory, Chaudhry and Meroney (5) have shown that

$$\frac{d\bar{z}}{dt} = ku_{*}/\phi(\bar{z}/L) \tag{3}$$

where ϕ is also unity for adiabatic conditions and describes the dependence on thermal stability of the vertical eddy diffusivity of the contaminant,

$$K = u_{*}kz/\phi(z/L) \quad . \tag{4}$$

Combination of (2) and (3) leads to

$$\bar{x} = \frac{1}{u_{*}k}\int_{z_0}^{\bar{z}} u(cz)\phi(z/L)\, dz \quad . \tag{5}$$

Chaudhry and Meroney use ϕ_h in (4) and (5), following the suggestion of Monin and Yaglom (8) that the eddy diffusivities of heat and a passive substance are equal. This choice is supported by their comparison of the predicted $\bar{z}$ with that measured 100 m downwind of the source during the

Prairie Grass SO_2 diffusion experiments. It is also supported by Crawford (9) and Dyer and Hicks (10), who found that the eddy transfer mechanisms of heat and water vapor were the same, by Galbally (11), who came to a similar conclusion for the transfer of heat and ozone, and by Sinclair et al (12) for heat, water vapor and carbon dioxide. Nieuwstadt and van Ulden (13), however, have recently found that numerical solutions of the diffusion equation produce comparable agreement with the 100 m Prairie Grass data using either ϕ_h or ϕ_m/α, where α is the value of ϕ_m/ϕ_h for neutral stratification.

By assuming a vertical distribution of the material equal to

$$\chi(x,z) = \chi(x,z=0)\ F(z/\bar{z},\ \bar{z}/L) \quad , \tag{6}$$

the crosswind-integrated concentration $\chi(x,z)$ may also be predicted from Lagrangian similarity theory (8). However, Malhotra and Cermak (14), simulating atmospheric diffusion from a surface source in a wind tunnel for both neutral and unstable thermal stratification, found that the effect of instability was to increase the scale of the diffusion without altering the form of the diffusing plume. Hence the influence of $\bar{z}/L$ on F appears to be quite weak.

Malhotra and Cermak's data fit the form

$$\chi(x,z) = \chi(x,z=0)\ \exp\left[-(z/b\bar{z})^r\right] \quad , \tag{7}$$

with a value of $r = 1.4$ appropriate to both neutral and unstable conditions. Pasquill (7) reports that for neutral conditions a value of $r = 1.15$ was found 100 m downwind of the source during 7 tracer releases at Porton, England, and a value of 1.5 was found at 229 m during 29 releases at Cardington, England. Elliot (15) has investigated the vertical distribution of tracer measured during Prairie Grass at 100 m downwind of the source and reported an average value of $r = 1.5$ for the 41 releases analyzed. He found that a Gaussian value of 2 for r is an overestimate except for fairly stable thermal stratification, that 1.5 was more appropriate for near-neutral conditions, and that r was less than 1.5 for unstable stratification. Analyzing the same data, Nieuwstadt and van Ulden (13) found values of 2.0, 1.3, and 1.0 for stable, neutral and unstable stratification, respecitvely.

The constant b of Eq. (7) is determined from the definition of $\bar{z}$,

$$\bar{z} = \int_0^\infty z\chi(x,z)dz \bigg/ \int_0^\infty \chi(x,z)\, dz \quad , \tag{8}$$

to be equal to $\Gamma(1/r)/\Gamma(2/r)$, where Γ is the gamma function. $\chi(x,z=0)$ is determined by the continuity condition

$$\int_0^\infty u(z)\chi(x,z)\, dz = Q \quad . \tag{9}$$

Substituting (7) into (9) and putting the result in dimensionless form,

$$\left[\frac{u_* z_0}{k} \; \frac{\chi(x,z=0)}{Q}\right]^{-1} = \int_1^\infty \left[f(z/L) - f(z_0/L)\right] \times \exp\left[-(z/b\bar{z})^r\right] d(z/z_0) \tag{10}$$

where f is a dimensionless function describing the wind profile,

$$u(z) = \frac{u_*}{k}\left[f(z/L) - f(z_0/L)\right] \quad . \tag{11}$$

Finally, the constant c in (2) is determined by calculating the mean advection velocity,

$$u(c\bar{z}) = \int_0^\infty u(\bar{z})\chi(x,z)\, dz \bigg/ \int_0^\infty \chi(x,z)\, dz \quad . \tag{12}$$

Again using (7),

$$u(c\bar{z}) = \left[\frac{\bar{z}\;\chi(x,z=0)}{Q} \; \frac{\Gamma^2(1/r)}{r\,\Gamma(2/r)}\right]^{-1} , \tag{13}$$

which may be evaluated with the aid of (10).

The quantity $u_* z_o \chi(x,z=0)/kQ$ has been calculated as a function of x/z_o and z_o/L from (5), (10) and (13). Businger et al's (16) formulas for ϕ_h and ϕ_m have been used, along with Paulson's (17) integral of the Businger et al formula for ϕ_m to get f:

$$\left.\begin{aligned} \phi_h(\zeta) &= 0.74 + 4.7\zeta \\ \phi_m(\zeta) &= 1 + 4.7\zeta \\ f(\zeta) &= \ln + 4.7\zeta \end{aligned}\right\} \zeta \geq 0$$

$$\left.\begin{aligned} \phi_h(\zeta) &= 0.74\ (1-9\zeta)^{-1/2} \\ \phi_m(\zeta) &= (1-15\zeta)^{-1/4} \\ f(\zeta) &= \ln\zeta - 2\ \ln[(1+\psi)/2] + \\ &\quad \ln[(1+\psi^2)/2] - 2\ \tan^{-1}\psi \end{aligned}\right\} \zeta \leq 0$$

where $\zeta = z/L$, $\psi = (1-15\ \zeta)^{1/4}$ and $k = 0.35$. Calculations have been made with ϕ equal to ϕ_h, ϕ_m and ϕ_m/α; with $r = 1$, 1.5 and 2; and also using an alternate formula for $\bar{z}$ as a function of x proposed by van Ulden (1978). In the following section these predictions are compared to data from the Prairie Grass experiments.

3. Comparisons with Observations

During Project Prairie Grass (18), tracer concentrations were measured at a height of 1.5m along arcs at distances of 50m, 100m, 200m, 400m, and 800m from the source. These ground-level measurements were summed along each arc and divided by the source strength to give the normalized CWIC at each downwind distance. Concurrent vertical profiles of wind speed and temperature were used to estimate L and u_* for each diffusion experiment. Second-order polynomials in ln z were first fit to the profiles by a least-squares technique, and the gradient Richardson number was calculated at several heights from the fitted profiles and converted to z/L using

$$z/L = \phi_m^2 Ri/\phi_h \tag{14}$$

and the empirical formulas for ϕ_h and ϕ_m. The friction velocity was then calculated by a least-squares fit of the empirical wind profile function f to the measured wind profile, using the value of L previously calculated for a height of 2 m and a roughness length z_o = 0.6 cm.

In Figs. 1-4 the observed $u_*\chi(x,z=1.5m)/Q$ are plotted as a function of thermal stability parameterized by 1/L. The open circles denote cases where the computed L varied by more than a factor of 2 between the heights of 1 m and 4 m, indicating that the empirical formulas for ϕ_m and ϕ_h were not compatible with the observed profiles of wind and temperature. This occurs mostly for strongly stable stratification when the surface flux layer may be quite shallow compared to the height of the profile measurements and the vertical extent of the diffusing plume.

Eddy Diffusivity

Fig. 1 compares the data at 400m with Lagrangian similarity prediction using r = 1.5 and $\phi = \phi_h$, ϕ_m and ϕ_m/α. A similar comparison is found at all distances. While the predictions are little different for strongly stable conditions, the superiority of ϕ_h is quite obvious for near-neutral and unstable thermal stratifications. ϕ_m/α is a good predictor only near neutral stability where it matches ϕ_h by definition.

Vertical Distribution

The predictions of $u_*\chi/Q$ are not as sensitive to the value of r. Figs. 2 and 3 compare the data at 100m and 800m with Lagrangian similarity predictions using $\phi = \phi_h$ and r = 1 and 2. The curve for r = 1.5 is intermediate and lies closer to the curve for r = 2, predicting values 10% to 15% greater than the r = 2 curve at 800m.

A comparison of these data with the Lagrangian similarity predictions does not indicate an increase of r with increasing stability. More noticeable is a change from r = 1.5 to r = 2 with increasing distance. At 50m and 100m the predictions for $r = 1.5$ are best, in agreement with Elliot's (15) average value determined from the elevated tracer measurements at 100m. At 200m the predictions for $r = 1.5$ and $r = 2$ are equally good, and at 400m and 800m the predictions for $r = 2$ are best. A value of $r = 1$ gives the poorest fit to the data at all distances.

An Alternate Relation Between $\bar{z}$ and x

Applying the same technique used by Chaudhry and Meroney (5), van Ulden (6) recently proposed the relation

$$x = \frac{1}{u_* k} \int_{z_o}^{\bar{z}} u(p\bar{z})\phi(p\bar{z}/L)dz, \tag{15}$$

with $p = 1.55$, to replace (5). Eqs. (5) and (15) can both result from the same approach because they are both approximate solutions based on slightly different assumptions. A choice between the two must finally be based on a comparison with observations.

Fig. 4 compares the Prairie Grass data at 200m to the predictions of (5) and (15) with $\phi = \phi_h$ and $r = 1.5$. A similar comparison is found at all distances. Eq. (15) is better than (5) for strongly stable and unstable conditions where the data are fewer, more scattered and (on the stable side) less reliable. However for near-neutral stability, $-.05<1/L<.05$, Eq. (15) overpredicts $u_* \chi/Q$ and Eq. (5) is clearly better. For neutral stability, $\phi = 1$ and the only difference between the equations is the choice of the advecting wind. Since $c = 0.63$ for $r = 1.5$, Eq. (15) specifies a wind speed at more than double the height, causing $\bar{z}$ to be low and $u_* \chi/Q$ to be high.

4. Conclusions

Several alternate Lagrangian similarity predictions have been compared with the ground-level, crosswind-integrated tracer concentration data from the Prairie Grass atmospheric diffusion experiments. Very good comparisons with the data were obtained with the assumption that the eddy diffusivity of a passive contaminant is equal to K_h and for values of the exponent r in the vertical distribution equal to either 1.5 or 2. Noticeably poorer comparisons were found with either r = 1 or the assumption of an eddy diffusivity equal to K_m or αK_m, where α is the neutral value of K_h/K_m. The ground-level data did not indicate a dependence of the exponent on thermal stability. Two forms of the Lagrangian similarity relations for $\bar{z}$ were tested. Chaudhry and Meroney's (5) equation,

$$d\bar{z}/dx = K(\bar{z})/\bar{z}u(c\bar{z}) \quad , \tag{16}$$

was found to provide a better overall fit to the data than van Ulden's (6) equation,

$$d\bar{z}/dx = K(p\bar{z})/p\bar{z}u(p\bar{z}) \quad , \tag{17}$$

particularly in near-neutral conditions where the latter equation noticeably overpredicts $u_*\chi/Q$.

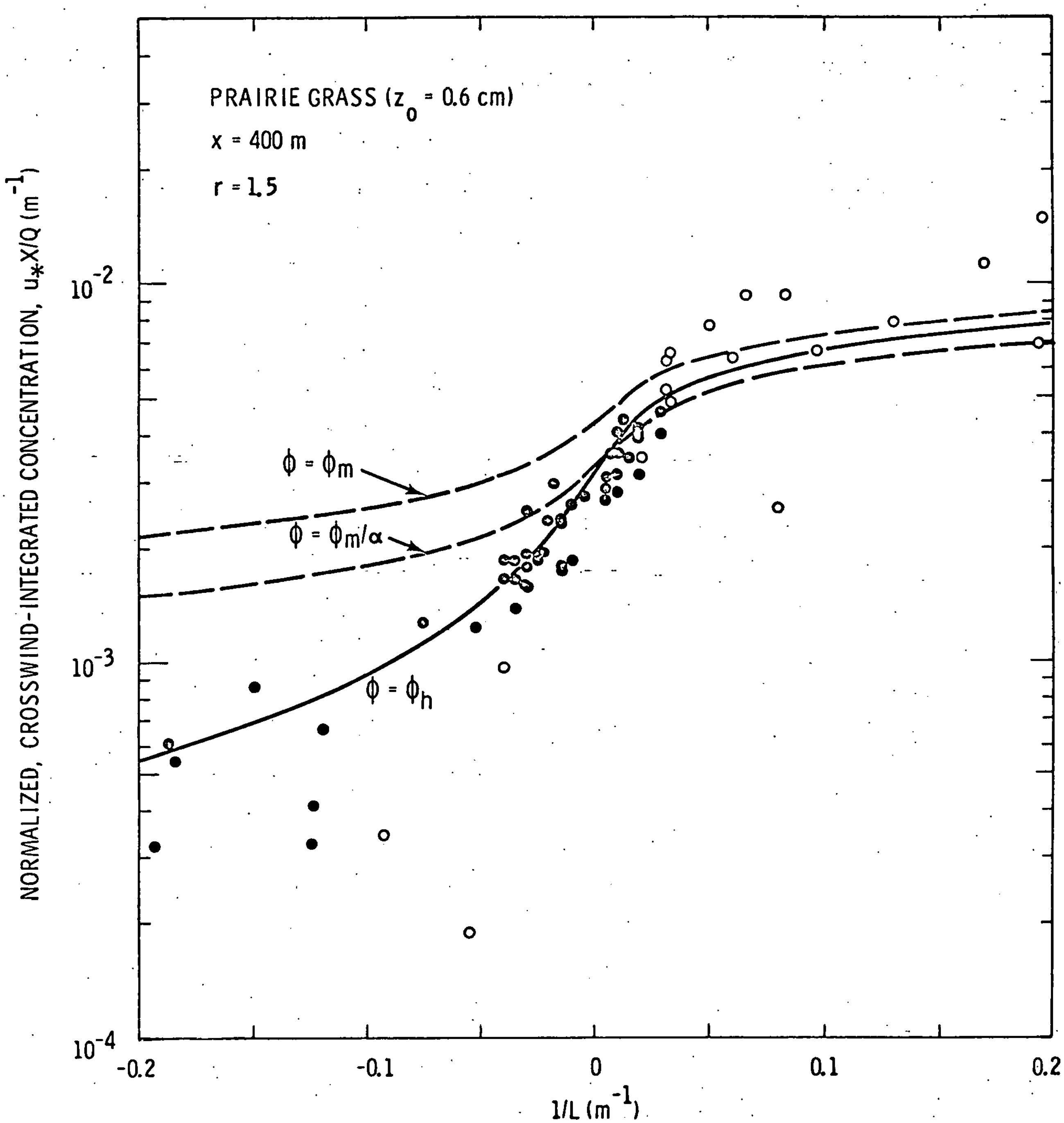

Figure 1. Measured contaminant concentrations 400m downwind of the source compared to predictions for several choices of eddy diffusivity.

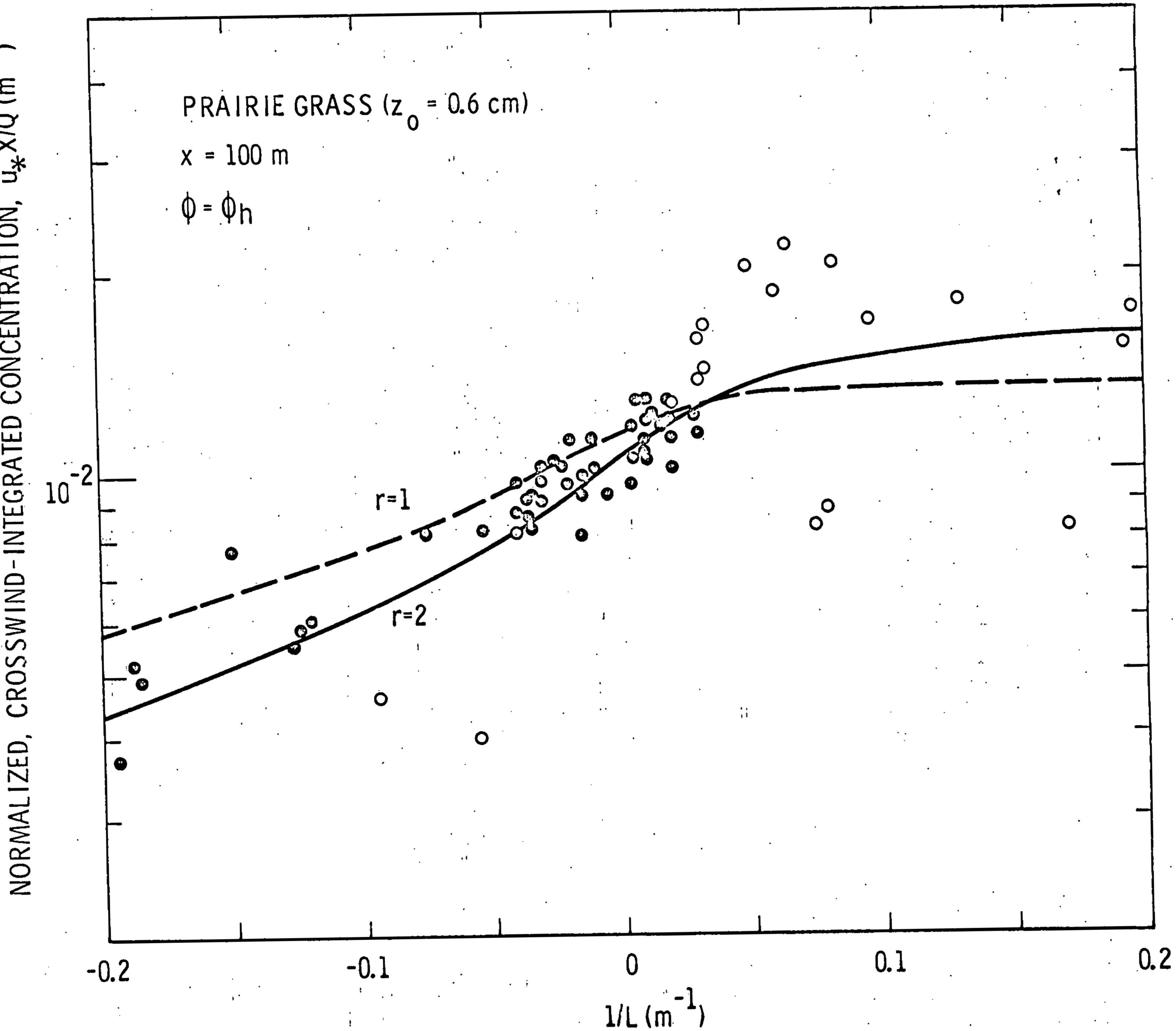

Figure 2. Measured contaminant concentrations 100m downwind of the source compared to predictions for two vertical distributions.

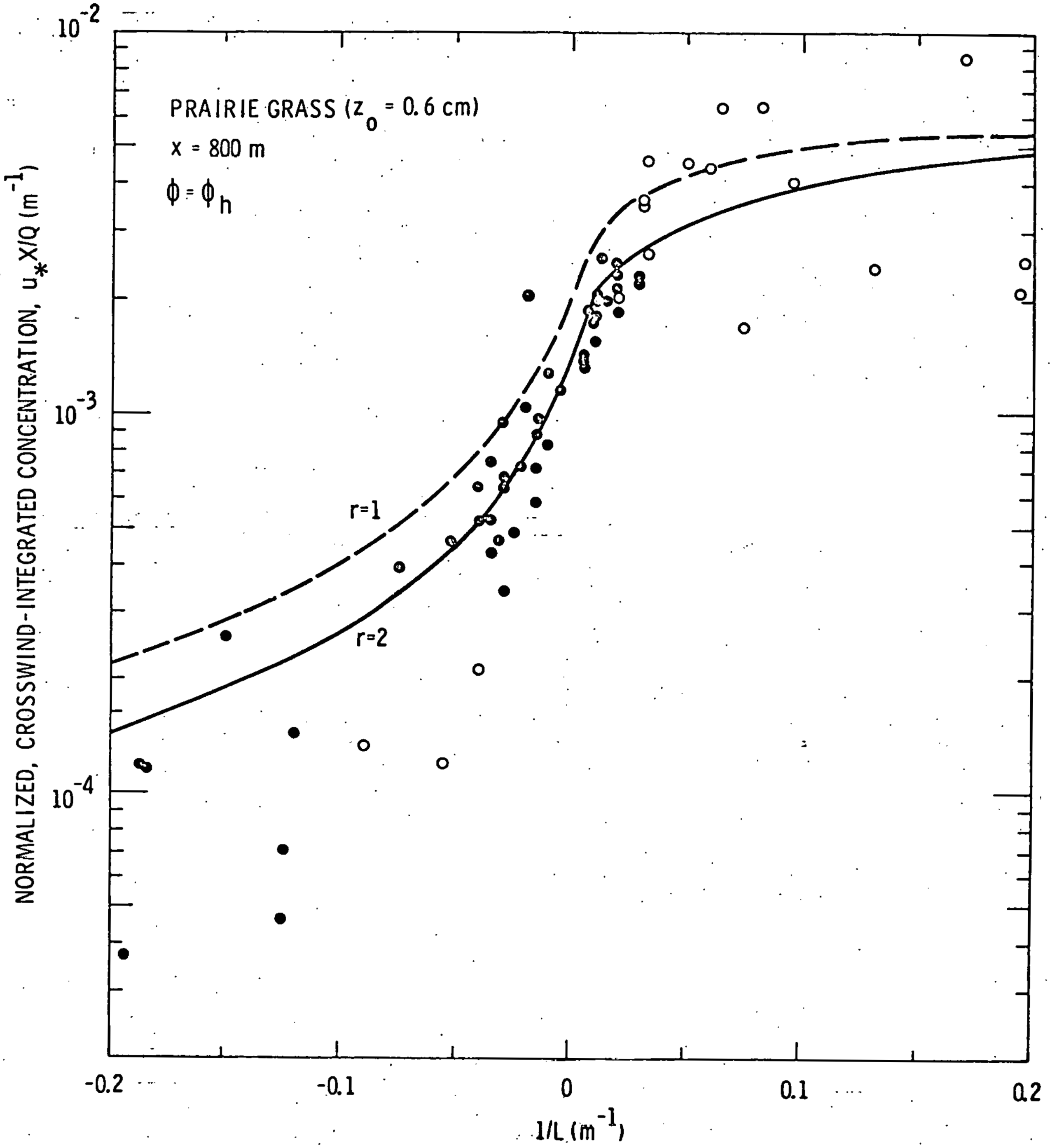

Figure 3. Measured contaminant concentrations 800m downwind of the source compared to predictions for two vertical distributions.

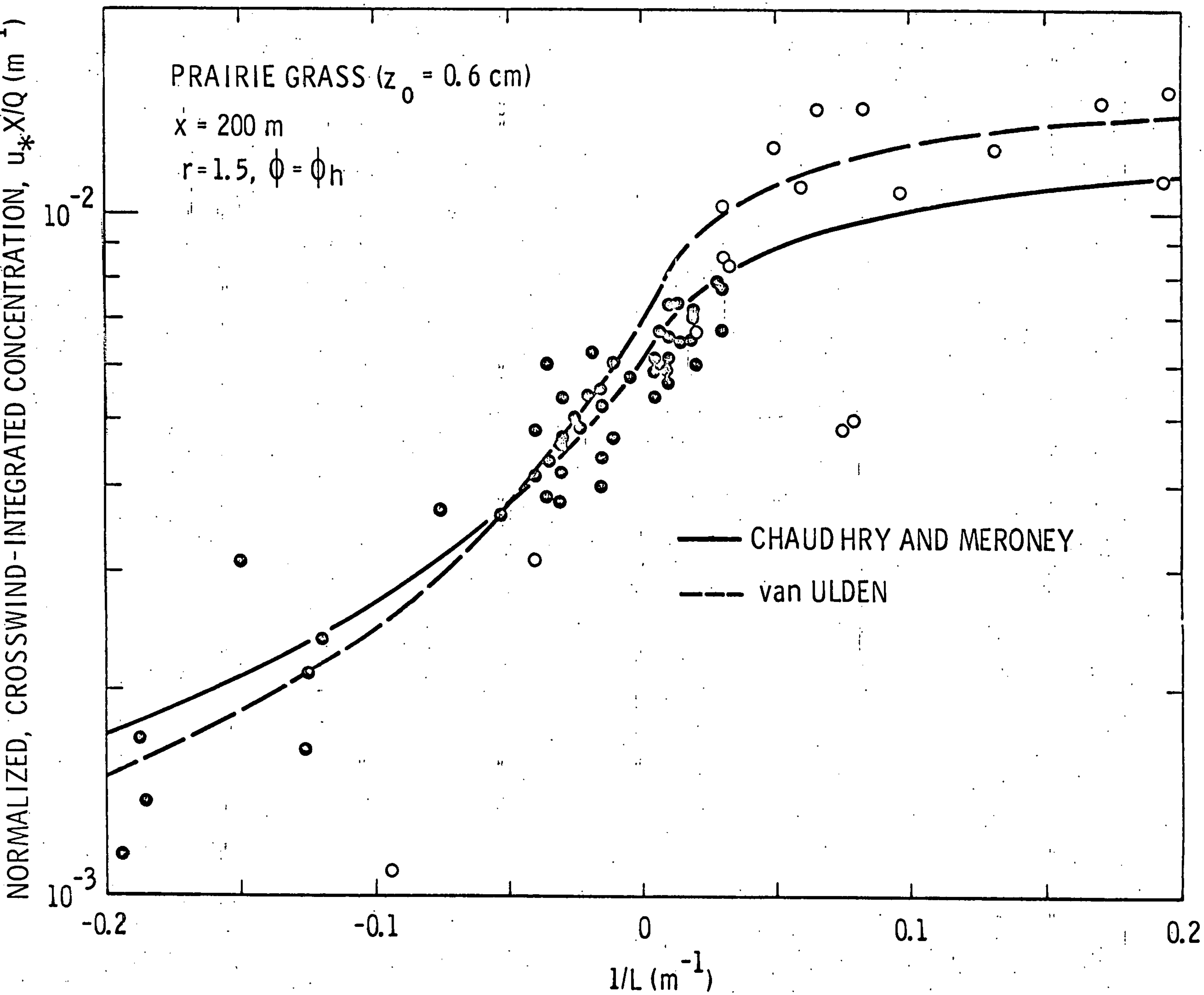

Figure 4. Measured contaminant concentrations 200m downwind of the source compared to predictions for alternate relations between $\bar{z}$ and x.

Acknowledgments

This work was supported by the U.S. Department of Energy and the U.S. Nuclear Regulatory Commission under Contract EY-76-C-06-1830.

References

1. Monin, A.S., "Smoke Propagation in the Surface Layer," Advances in Geophysics, 6, pp. 331-341, 1959.

2. Batchelor, G.K., "Diffusion from Sources in a Turbulent Boundary Layer," Archiwum Mechaniki Stosowanej, 3, pp. 661-670, 1964.

3. Elison, T.H., "Turbulent Diffusion," Sci. Progress, 47, pp. 495-506, 1959.

4. Chatwin, P.C., "The Dispersion of a Puff of Passive Substance in the Constant-Stress-Region," Quart. J. Roy. Meteor, Soc., 94, pp. 401-441, 1968.

5. Chaudhry, F.H. and Meroney, R.N., "Similarity Theory of Diffusion and the Observed Vertical Spread in the Diabatic Surface Layer," Bound. Layer Meteor., 3, pp. 405-415, 1973.

6. van Ulden, A.P., "Simple Estimates for Vertical Diffusion from Sources near the Ground," Atm. Environ., 12, pp. 2125 - 2129, 1978.

7. Pasquill, F., Atmospheric Diffusion, 2nd Ed., John Wiley and Sons, New York, 1974.

8. Monin, A.S. and Yaglom, A.M., Statistical Hydromechanics, Hauka Press, Moscow, 1965.

9. Crawford, T.V., "Moisture Transfer in Free and Forced Convection," Quart. J. Roy. Meteor. Soc., 91, pp. 18-27, 1965.

10. Dyer, A.J. and Hicks, B.B., "Flux-Gradient Relationships in the Constant Flux Layer," Quart. J. Roy. Meteor. Soc., 96, pp. 715-721, 1970.

11. Galbally, I.E., "Ozone Profiles and Ozone Fluxes in the Atmospheric Surface Layer," Quart. J. Roy. Meteor. Soc., 97, pp. 18-29, 1971.

12. Sinclair, T.R., Allen, Jr., L.H., and Lemon, E.R., "An Analysis of Errors in the Calculation of Energy Flux Densities Above Vegetation by a Bowen-Ratio Profile Method," Bound. Layer Meteor., 8, pp. 129-140, 1975.

13. Nieuwstadt, F.T.M., van Ulden, A.P., "A Numerical Study on the Vertical Dispersion of Passive Contaminants from a Continuous Source in the Atmospheric Surface Layer," Atm. Environ., 12, pp. 2119-2124, 1978.

14. Malhotra, R.C. and Cermak, J.E., "Mass Diffusion in Neutral and Unstably Stratified Boundary-Layer Flows," Int. J. Heat Mass Transfer, 7, pp. 169-186, 1964.

15. Elliot, W.P., "The Vertical Diffusion of Gas from a Continuous Source," Int. J. Air Water Poll., 4, pp. 33, 1961.

16. Businger, J.A., Wyngaard, J.C., Izumi, Y., and Bradley, E.F., "Flux-Profile Relationships in the Atmospheric Surface Layer," J. Atmos. Sci., 28, pp. 181-189, 1971.

17. Paulson, C.A., "The Mathematical Representation of Wind Speed and Temperature Profiles in the Unstable Atmospheric Surface Layer," J. Appl. Meteor., 9, pp. 857-861, 1970.

18. Barad, M.L., ed, "Project Prairie Grass, A Field Program in Diffusion," Geophysical Research Paper No. 59, Vols. I and II, AFCRC-TR-58-235, Air Force Cambridge Research Center, Bedford, MA, 1958.