FOOTPRINT PREDICTION OF SCALAR FLUXES USING A MARKOVIAN ANALYSIS

M. Y. LECLERC*

Department of Plant, Soil and Biometeorology, Utah State University, Logan, UT 84322, U.S.A.

and

G. W. THURTELL

Department of Land Resource Science, University of Guelph, Guelph, Ontario, Canada, N1G 2W1.

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Abstract. The contribution of upwind sources to measurements of vertical scalar flux density as a function of fetch ('footprint') is predicted using a Markovian simulation of fluid particle trajectories. Results suggest that both footprint peak position and magnitude change dramatically with surface roughness, thermal stability and observation levels. Results also indicate that the much used 100 to 1 fetch-to-height ratio grossly underestimates fetch requirements when observations are made above smooth surfaces, in stable conditions or at high observation levels.

1. Introduction

A knowledge of the spatial extent and relative importance of upwind source areas to downwind fluxes ("footprint") observed at height z for different atmospheric stabilities and surface roughnesses, is important since many sites fall short of the ideal requirement of horizontal homogeneity. Localized sources of biogenic gases such as isoprene and methane, pesticide volatilization from treated fields, evaporation from locally irrigated crops, 'hot spots' caused by differences in albedo or surface thermal properties, and the sea-land interface are just a few examples of horizontal inhomogeneity leading to local advection. Largely because of a lack of more rigorous criteria, the 100 to 1 fetch-to-height ratio is used to ensure that sensors are placed within the internal boundary layer (IBL) of a limited source area. The thickness of the IBL grows with instability, relaxing fetch requirements in convective conditions. Conversely, the footprint expands in stable conditions. However, the specific effects of thermal stability and surface roughness on the development of the IBL have been poorly documented. Figure 1 from Tanner (1988) illustrates the sensitivity of flux measurements to horizontal surface inhomogeneities. Bowen ratio values for two independent systems were formed using sensible heat and latent heat fluxes measured with eddy-correlation techniques. The underlying surface was a wet smooth soil littered with downed wheat stubble extending 170 m upwind to a soybean field approximately 40 cm high. When both systems were placed at the same height (1.35 m, day 2), Bowen ratio values agreed well with one another. However, when system 1 was lowered to 90 cm (day 3),

* Corresponding address: M. Y. Leclerc, Dept. of Physics, University of Quebec in Montreal, C.P. 8888 Succ. A, Montreal, Que, Canada H3C 3P8.

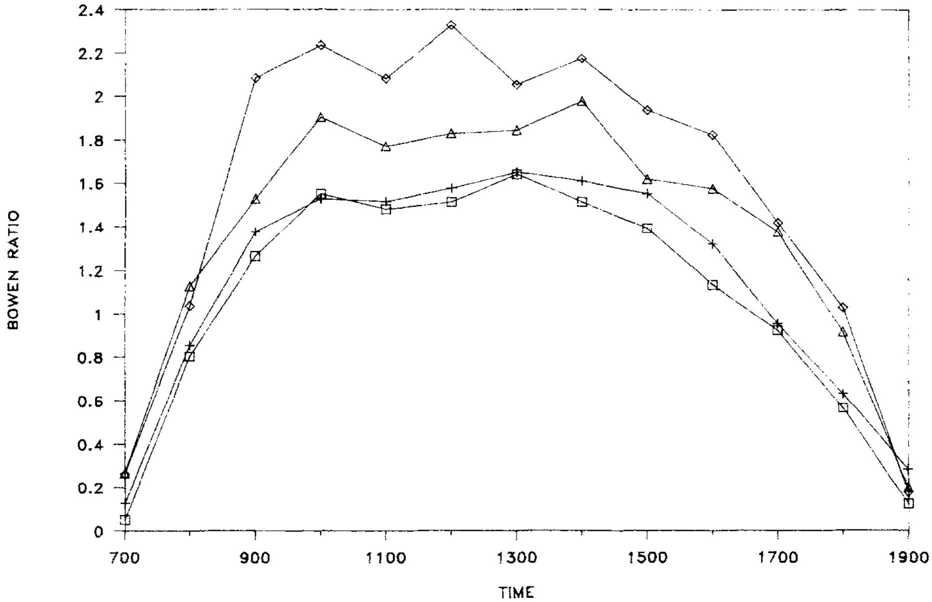

Fig. 1. Bowen ratios obtained with two eddy-correlation systems: (day 2) EC1 □; EC2 +; (day 3) EC1 ◇; EC2 △.

system 2 showed relatively lower Bowen ratio values because of the greater latent heat flux from the soybean field observed at the 1.35 m height.

This paper illustrates the relative importance of source regions upwind from the point of observation by presenting the effective 'footprints' and their dependence on thermal stability, surface roughness and observation levels. This paper also describes the theory and methods used in the simulations of footprints and discusses the reliability and implications of these results to those planning field measurement campaigns. A companion paper (Schuepp *et al.*, 1990) has compared simple approximate analytical solutions of the diffusion equation in near-neutral conditions against these present predictions.

2. Historical Perspective

Analytical and numerical solutions to diffusion equations abound in the literature for many source configurations, initial and boundary conditions and levels of idealization of diffusivity and velocity profiles (Deacon, 1949; Calder, 1952; Sutton, 1953; Philip, 1959; Dyer, 1963; Taylor, 1970; Rao *et al.*, 1974; Wilson, 1982; Horst and Slinn, 1984). From these solutions, vertical scalar flux profiles are obtained as a function of downwind distance. Conversely, the upwind 'footprint' of a local flux observation at height z can be determined in principle.

Although analytical solutions have become increasingly refined, their ability to reproduce the diffusion process correctly is limited in many cases. Present analytical solutions for ground-level releases require a generally smooth surface, precluding their use above very rough orchard or forest canopies. Furthermore, these solutions predict the maximum in the vertical concentration profile to occur at the surface when a plume is travelling downwind from a surface line source; this is in sharp contrast with Willis and Deardorff's findings (1976) from convective boundary-layer tank experiments. Most of these solutions also ignore both the effect of atmospheric stability on the flow field and the change in diffusivity with height. A notable exception is the work of Horst and Slinn (1984) whose predictions compared well with experimental results in near-neutral conditions. However, the discrepancy between their solution and experiments grew as stability departed from neutral conditions. Their analytical solution is also awkward to use because it requires the inclusion of ill-defined constants.

Given these limitations, we felt that an alternative method should be sought. Stochastic modelling of atmospheric diffusion presents few of the drawbacks mentioned above and for simple cases, predictions have been in general agreement with available tracer experiments (Wilson *et al.*, 1981b). These simulations can provide also a preliminary benchmark against which physically simplified analytical solutions (Schuepp *et al.*, 1990) can be evaluated.

3. Lagrangian Analysis of Scalar Transfer

This simulation assumes a steady-state two-dimensional flow where streamwise velocity fluctuations (much smaller than the mean wind speed) are neglected. It considers the diffusion of a passive tracer which does not adhere to the surface or recombine with other molecules in the atmosphere, in a shear flow with vertically inhomogeneous Gaussian turbulence. The assumption of Gaussian turbulence is reasonable in the surface layer where the skewness of the vertical velocity is small. The present stochastic simulation specifically addresses the effects of roughness elements and buoyancy on plume dispersion but does not include any step-changes in surface roughness or scalar properties.

The Lagrangian stochastic approach to turbulent dispersion is well known and will only be briefly described. Readers are referred to Sawford (1985) for an exhaustive review. The diffusion of an inert scalar can be modelled by numerically constructing an ensemble of particle trajectories from a stochastic differential equation (the Langevin equation), which determines the evolution of a Lagrangian trajectory in space-time. This approach has been applied to dispersion in inhomogeneous turbulence within the surface layer (Reid, 1979; Wilson *et al.*, 1981a; Wilson *et al.*, 1983), inside vegetation (Raupach *et al.*, 1986; Leclerc *et al.*, 1988) and in the convective boundary layer (Thomson, 1984; de Baas *et al.*, 1986; Sawford and Guest, 1987).

We consider vertical dispersion by turbulent mixing and horizontal dispersion downwind by horizontal advection. In high Reynolds number flow, the Lagrangian vertical velocity of a single particle in the ensemble, $W(t)$, is well approximated by that of a Markov process (Sawford, 1984) so that $W(t)$ satisfies the linear stochastic differential equation of the form

$$\mathrm{d}w = (aW + b)\mathrm{d}t + \mathrm{d}R. \tag{1}$$

The deterministic coefficients a and b depend on height z of a single particle; t is the diffusion time, and R is a random process. For the case of inhomogeneous turbulence, following both Wilson *et al.* (1983) and an analysis of that method by Thomson (1984) and Sawford (1986), a dimensionless time series is formed

$$\tilde{W}(t) = \alpha\tilde{W}(t) + \beta r \tag{2}$$

where r is a random number with unit variance and a Gaussian distribution. For small time steps, the Markov chain above generates a series with an exponential autocorrelation function $\exp(-\Delta t/\tau_L)$, where Δt is the time step and $\tau_L(z)$ is the Lagrangian time scale over which instantaneous velocities are correlated. We chose the time step $\Delta t = 0.1\tau_L$, making α a constant. After several arithmetic manipulations, it can be shown that $\beta = (1 - \alpha^2)^{0.5}$ to ensure that turbulent energy is conserved over time. The dimensionless velocities are then rescaled as turbulent vertical velocities such that the instantaneous vertical velocity becomes

$$W = \tilde{W}\sigma_w \tag{3}$$

where σ_w is the root-mean-square value of the vertical velocity. The flow field is described by the turbulent vertical velocity σ_w, the mean horizontal wind speed $\bar{u}(z)$, and the Monin–Obukhov length L. The Lagrangian turbulence length and time scales of the turbulent vertical velocities are assumed to be self-similar about the z-axis i.e., $\Lambda = \Lambda(z)$, $\tau_L = \tau_L(z)$. In unstable and in stable conditions, σ_w is a function of height and we bias the trajectories following the technique used by Leclerc *et al.* (1988) in which the probability of reflection is calculated based on the gradient in the variance of the vertical velocity. The mean wind profile used (Dyer and Hicks, 1970) is a function of atmospheric stability. For $L < 0$, the mean horizontal windspeed is

$$\bar{u}(z) = \frac{u_*}{k}\left[2\arctan\Phi_m^{-1} + \ln\left(\frac{\Phi_m^{-1} - 1}{\Phi_m^{-1} + 1}\right) - f(z_0)\right] \text{ and} \tag{4}$$

u_*, k and z_0 are the friction velocity, the Von Karman constant (assumed to be 0.4) and the roughness length respectively,

$$\Phi_m = \left(1 - 16\frac{z}{L}\right)^{-1/4} \tag{5}$$

$$f(z_0) = 2\arctan\Phi_{m0}^{-1} + \ln\left(\frac{\Phi_{m0}^{-1} - 1}{\Phi_{m0}^{-1} + 1}\right). \tag{6}$$

Φ_{m0} is a function of $\Phi_m(z_0/L)$.

In stable conditions ($L > 0$),

$$\Phi_m = 1 + 4.7\frac{z}{L} \text{ (Businger } et\ al.\text{, 1971)} \tag{7}$$

and $\tilde{u}(z)$ becomes

$$\tilde{u}(z) = \frac{u_*}{k}\left[\ln\frac{z}{z_0} + 4.7\left(\frac{z - z_0}{L}\right)\right]. \tag{8}$$

The turbulence velocity scales used for $0 < L \leqslant +\infty$ (Haugen, 1973) were

$$\sigma_w = 1.25u_* \tag{9}$$

while for $L < 0$ (Wilson *et al.*, 1982),

$$\sigma_w = 1.25u_*\left(1 + 4.1\frac{z}{-L}\right)^{1/3}. \tag{10}$$

The Lagrangian time scale τ_L, for $L < 0$ is

$$\tau_L = \frac{0.5z\left(1 - 6\frac{z}{L}\right)^{1/4}}{\sigma_w(z)} \tag{11}$$

while for $L > 0$ it is equal to

$$\tau_L(z) = \frac{\left[\dfrac{0.5z}{\left(1 + 5\frac{z}{L}\right)}\right]}{\sigma_w(z)}. \tag{12}$$

For $L = \infty$, it becomes equal to

$$\tau_L(z) = \frac{0.5z}{\sigma_w(z)}. \tag{13}$$

Fluid particles are released at the surface from an infinite cross-wind strip and particles are counted through multiple downwind towers. The footprint is calculated by determining the contribution that each of the respective upwind sources made to the total vertical flux at each height. The summation of these contributions into a cumulative fractional flux from source areas with increasing upwind distance (fetch) approaches unity asymptotically.

4. Results

4.1. Footprints as a function of observation level

The relative contribution of a crosswind infinite source strip at the surface to the downwind scalar flux at observation levels from 3 to 75 m is presented in Figures

2 and 3. These footprints are expected above a short crop (approx. 50 cm high) in neutral conditions. Figure 2 showing flux contributions for 3 and 5 m heights is of particular interest in Bowen ratio applications where temperature and vapor pressure gradients are measured by placing sensors at two levels. The maximum

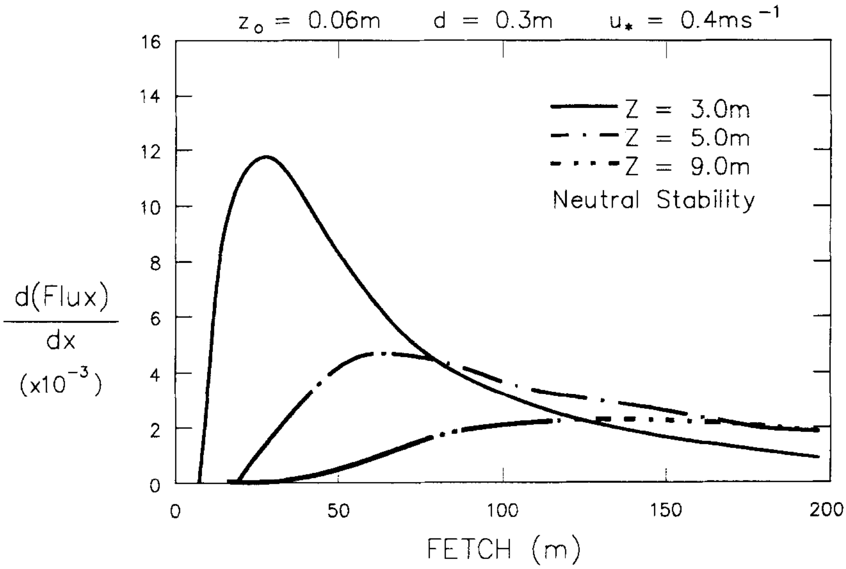

Fig. 2. Fraction of the vertical scalar flux density contributed by a crosswind infinite surface source strip as a function of downwind distance (footprint) for $z = 3.0$, 5.0 and 9.0 m.

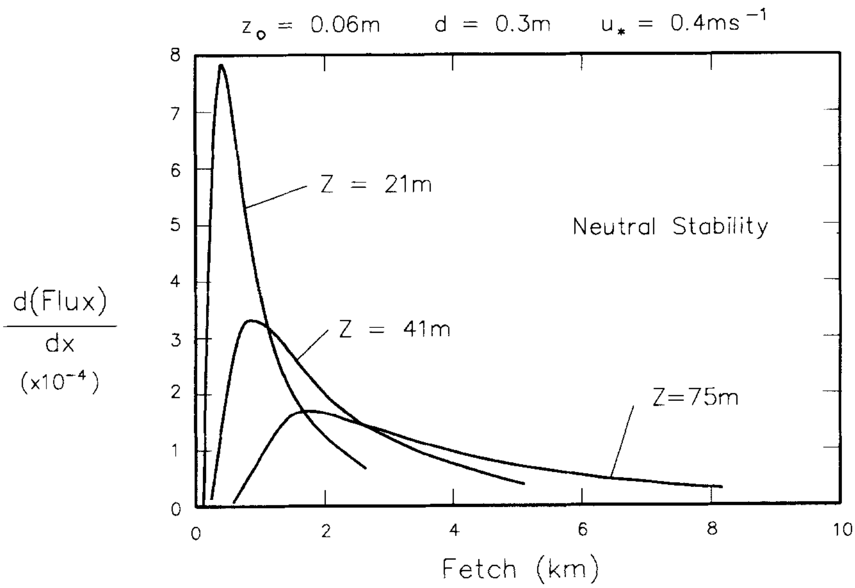

Fig. 3. Fraction of the vertical scalar flux density contributed by a crosswind infinite source strip at the surface as a function of downwind distance (footprint) for $z = 21$, 41 and 75 m.

flux contribution 'seen' by the lower sensors occurs closer to the point of observation but its magnitude is about three times as large as the peak in the footprints 'seen' by the higher sensors. Natural variability is inherent to field measurements, and experimental results might not agree perfectly with the results shown here. In addition, even though these simulations were performed using hundreds of thousands of particles and millions of random numbers, these results carry some uncertainty associated with the finite length of the random number series used.

For airborne flux measurements, the criterion of horizontal homogeneity is particularly difficult to fulfill. Depending on flight levels (21, 41, 75 m), the footprint over a short crop peaks at about 0.5, 1 and 2 km respectively (Figure 3), from the experimental platform. These implications are important because to this date, a theoretical basis suggesting the optimum flight altitude has not been brought forth. Additionally, the relevance of surface measurements used to validate aircraft observations should be re-evaluated since these results shed new light on the relative relevance of coincident surface and airborne flux observations. Figures 4 and 5 illustrate the asymptotic adjustment of flux with increasing fetch to equilibrium for typical ground level and aircraft observation levels. They are obtained by integrating the footprint functions presented above with respect to fetch length. The 100 to 1 fetch-to-height ratio rule clearly underestimates the fetch required for aircraft observation levels.

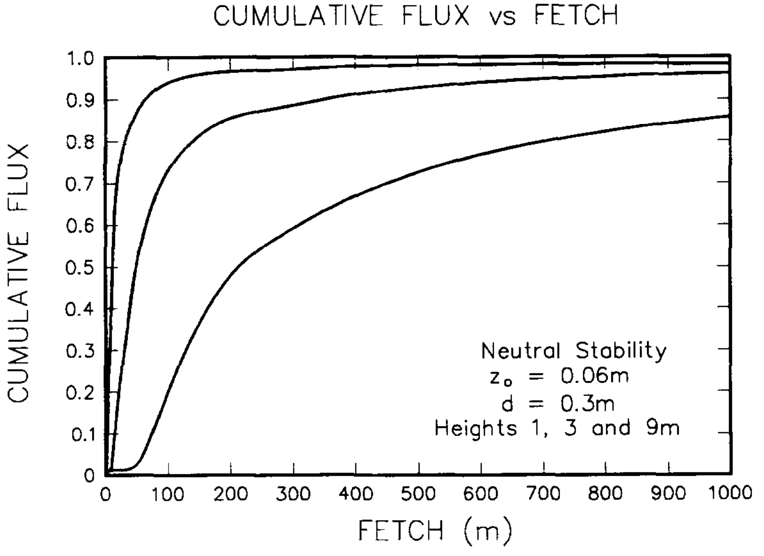

Fig. 4. Rate of adjustment of vertical scalar flux density with fetch ($u_* = 0.4$ m/s) for $z = 1$, 3 and 9 m, and $z_0 = 0.06$ m and $d = 0.3$ m.

4.2. Influence of Surface Roughness and Thermal Stability on Footprints and on the Rate of Flux Adjustment with Fetch

Figures 6 to 8 present the rate of flux adjustment with fetch for different observation levels and surface roughnesses. As expected, the smoother the surface, the weaker the vertical mixing, leading to a slower boundary-layer growth and greater

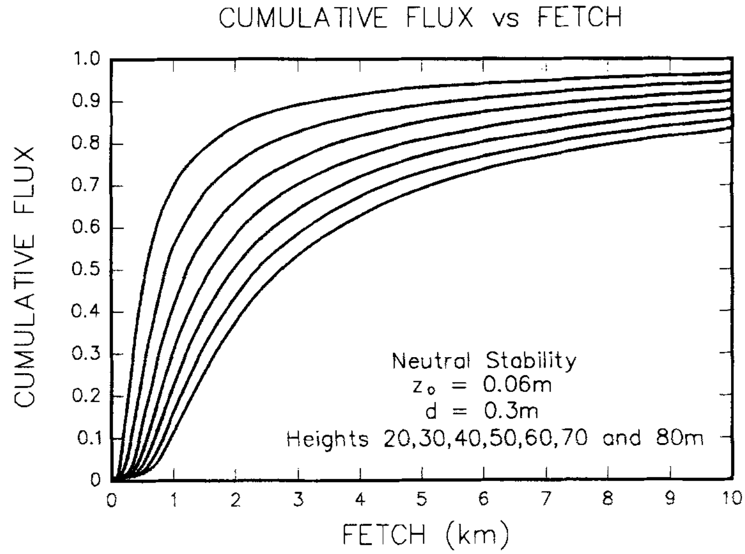

Fig. 5. Rate of adjustment of vertical scalar flux density with fetch ($u_* = 0.4$ m/s) for $z = 20$, 30, 40, 50, 60, 70 and 80 m, and $z_0 = 0.06$ m and $d = 0.3$ m.

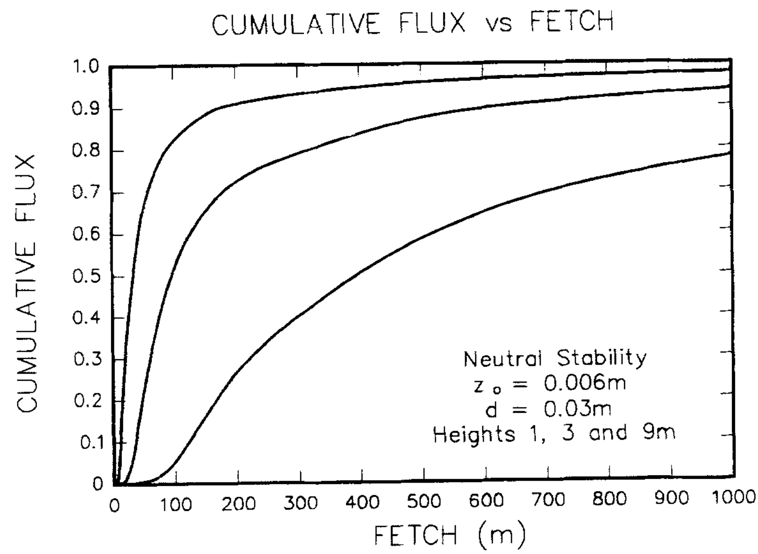

Fig. 6. Rate of adjustment of vertical scalar flux density with fetch ($u_* = 0.4$ m/s) for $z = 1$, 3 and 9 m, and $z_0 = 0.006$ m and $d = 0.03$ m.

fetch requirements. This is shown by comparing Figure 4 with Figure 6 and Figure 5 with Figures 7 and 8. Figure 9 summarizes the effect of surface roughness on the fetch where the peak in the footprint occurs as a function of observation level.

The sensitivity of footprint calculations to thermal stability is illustrated in Figure

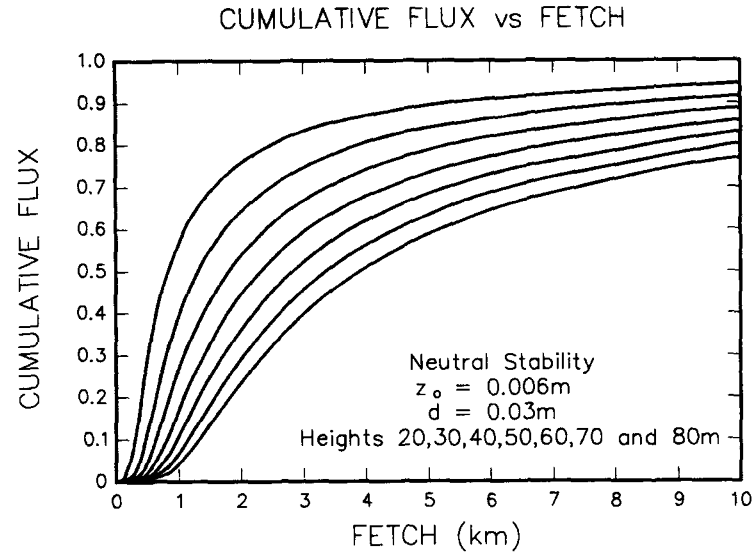

Fig. 7. Rate of adjustment of vertical scalar flux density with fetch ($u_* = 0.4$ m/s) for $z = 20$, 30, 40, 50, 60, 70 and 80 m, and $z_0 = 0.006$ m and $d = 0.03$ m.

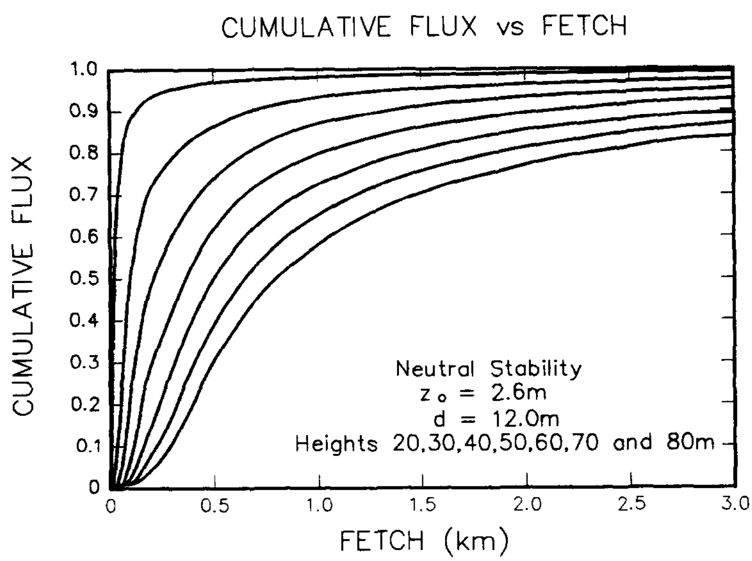

Fig. 8. Rate of adjustment of vertical scalar flux density with fetch ($u_* = 0.4$ m/s) for $z = 20$, 30, 40, 50, 60, 70 and 80 m, and $z_0 = 2.6$ m, and $d = 12.0$ m.

10. Far from the ground, buoyancy effects are prominent: at 11 m from the surface, the magnitude in the footprint peak in stable conditions ($L = +10$ m) is almost four times lower than in neutral conditions and six times lower than in unstable conditions ($L = -10$ m).

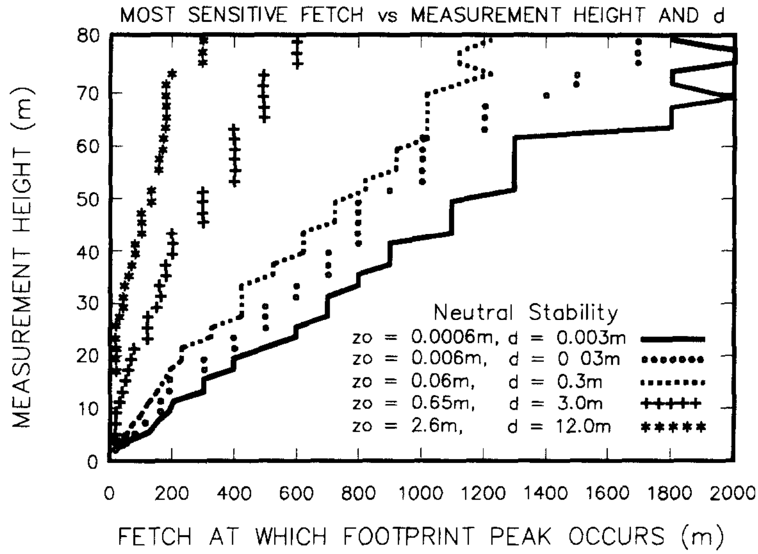

Fig. 9. Fetch at which footprint peak occurs.

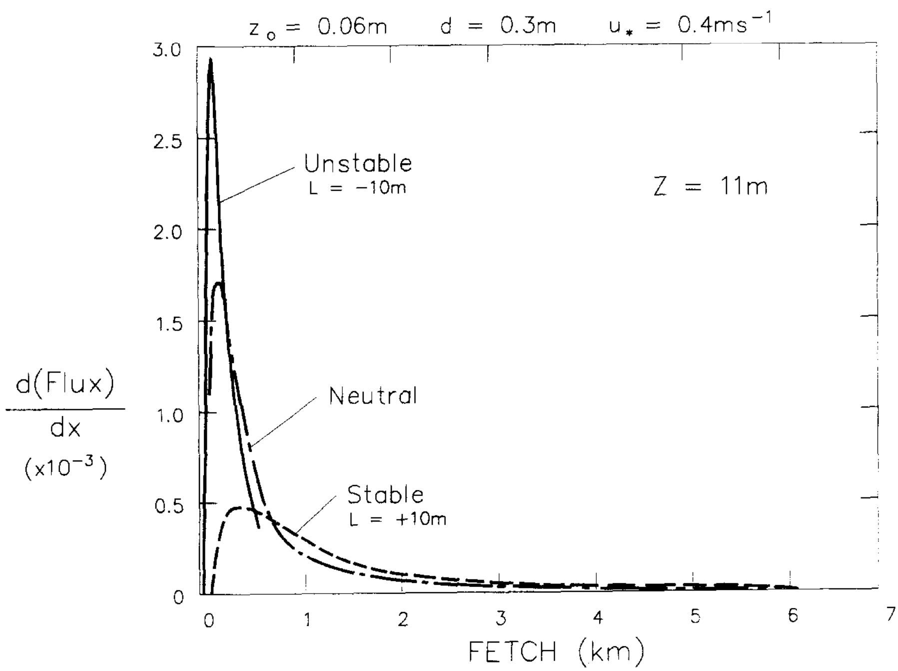

Fig. 10. Effect of thermal stability on footprints ($u_* = 0.4$ m/s) for $z = 11$ m, and $z_0 = 0.06$ m, $d = 0.3$ m.

5. Summary and Conclusions

This paper describes the Markovian simulation of the respective contribution of upwind sources to a point flux measurement at height z. Specifically, the prominent effects of surface roughness, thermal stability and observation levels on the upwind footprint are examined. These results are expected to be of interest to those planning future field measurement campaigns. Even though buoyancy effects are expected to be small near the ground, the 'footprint' for near-surface flux observations contracts in convective situations and expands in stable conditions. Measurements obtained during unstable daytime conditions represent fluxes from upwind surfaces closer to the point of observation than do those made during stable nighttime conditions. The 100 to 1 fetch-to-height ratio is shown to be adequate, albeit conservative for measurements made over tall, rough canopies such as forests because of the rapid growth of the IBL. This should encourage work over small forests otherwise thought to have inadequate fetch. Conversely, our results point out that for more commonly studied land sites with small surface roughness such as grass or short crops, the 100 to 1 ratio clearly underestimates the extent of upwind homogeneous surface needed.

Bowen ratio measurements are particularly sensitive to upwind surface inhomogeneities because of the different footprints seen by the upper and lower sensors. The extreme fetch needed for aircraft measurements may partially explain the typically poor correlation between simultaneous ground measurements and aircraft observations.

Additional research should include the modelling of footprints in the presence of step-changes in thermal stability and surface roughness. Further work is also needed in parameterizing turbulence statistics in highly unstable conditions where similarity theory fails. Finally, even though these simulations have a realistic basis, they should be validated by a field experiment.

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References

Businger, J. A., Wyngaard, J. C., Izumi, Y. and Bradley, E. F.: 1971, 'Flux Profile Relationships in the Atmospheric Surface Layer', *J. Atmos. Sci.* **25**, 1021–1025.

Calder, K. L.: 1952, 'Some Recent British Work on the Problem of Diffusion in the Lower Atmosphere', *Proc. U.S. Tech. Conf. Air Pollut.*, McGraw-Hill, New York, pp. 787–792.

Deacon, E. L.: 1949, 'Vertical Diffusion in the Lowest Layers of the Atmosphere', *Quart. J. Roy. Meteorol. Soc.* **75**, 89–103.

deBaas, A. F., van Dop, H. and Nieuwstadt, F. T. M.: 1986, 'An Application of the Langevin Equation for Inhomogeneous Conditions to Dispersion in a Convective Boundary Layer', *Quart. J. Roy. Meteorol. Soc.* **112**, 165–180.

Dyer, A. J.: 1963, 'The Adjustment of Profiles and Eddy Fluxes', *Quart. J. Roy. Meteorol. Soc.* **89**, 276–280.

Dyer, A. J. and Hicks, B. B.: 1970, 'Flux Gradient Relationships in the Constant Flux Layer', *Quart. J. Roy. Meteorol. Soc.* **96**, 715–721.

Haugen, D. A.: 1973, 'Workshop in Micrometeorology', American Meteorol. Soc., Boston, Massachusetts.

Horst, T. W. and Slinn, G. N.: 1984, 'Estimates for Pollution Profiles above Finite Area-Sources', *Atmos. Environ.* **18**, 1339–1346.

Philip, J. R.: 1959, 'The Theory of Local Advection: 1', *J. Meteorol.* **16**, 3–22.

Leclerc, M. Y., Thurtell, G. W. and Kidd, G. E.: 1988, 'Measurements and Langevin Simulations of Mean Tracer Concentration Fields Downwind from a Circular Line Source Inside an Alfalfa Canopy', *Boundary-Layer Meteorol.* **43**, 287–308.

Rao, K. S., Wyngaard, J. C. and Cote, O. R.: 1974, 'Local Advection of Momentum, Heat and Moisture in Micrometeorology', *Boundary-Layer Meteorol.* **7**, 331–348.

Raupach, M. R., Coppin, P. A. and Finnigan, J. J.: 1986, 'Experiments on Scalar Diffusion within a Plant Canopy Part 2. An Elevated Plane Source', *Boundary-Layer Meteorol.* **35**, 21–52.

Roberts, O. F. T.: 1923, *Proc. Roy. Soc.* (London), **A104**, 640.

Reid, J. D.: 1979, 'Markov Chain Simulations of Vertical Dispersion in the Neutral Surface Layer for Surface and Elevated Releases', *Boundary-Layer Meteorol.* **16**, 3–32.

Sawford, B. L.: 1984, 'Lagrangian Statistical Modelling of Turbulent Dispersion', *Proc. Eighth Int. Clean Air Conf.*, Melbourne, Clean Air Society of Australia and New Zealand, pp. 17–27.

Sawford, B. L.: 1985, 'Lagrangian Statistical Simulation of Concentration Mean and Fluctuation Fields', *J. Climate Appl. Meteorol.* **24**, 1152–1166.

Sawford, B. L.: 1986, 'Generalized Random Forcing in Random-Walk Turbulent Dispersion Models', *Phy. Fluids* **29**, 3582–3589.

Sawford, B. L. and Guest, F. M.: 1987, 'Lagrangian Stochastic Analysis of Flux-Gradient Relationships in the Convective Boundary Layer', *J. Atmos. Sci.* **44**, 1152–1165.

Schuepp, P. H., Leclerc, M. Y., MacPherson, J. I. and Desjardins, R. L.: 1990, 'Footprint Prediction of Scalar Fluxes from Analytical Solutions of the Diffusion Equation', *Boundary-Layer Meteorol.* **50**, 355–373.

Sutton, O. G.: 1953, *Micrometeorology: A Study of Physical Processes in the Lowest Layers of the Earth's Atmosphere*, McGraw Hill, London.

Tanner, B. D.: 1988, 'Use Requirements for Bowen Ratio and Eddy Correlation Determination of Evapotranspiration', *Proc. of the* 1988 *Specialty Conference of the Irrigation and Drainage Division*, ASCE Lincoln, Nebraska July 19–21.

Taylor, P. A.: 1970, 'A Model of Airflow above Changes in Surface Heat Flux, Temperature and Roughness for Neutral and Uns Conditions', *Boundary-Layer Meteorol.* **1**, 18–39.

Thomson, D. J.: 1984, 'Random Walk Modelling of Diffusion in Inhomogeneous Turbulence', *Quart. J. Roy. Meteorol. Soc.* **110**, 1107–1120.

Willis, G. E. and Deardorff, J. W.: 1976, 'A Laboratory Model of Diffusion into the Convective Planetary Boundary Layer', *Quart. J. Roy. Meteorol. Soc.* **102**, 427–445.

Wilson, J. D.: 1982, 'An Approximate Analytical Solution to the Diffusion Equation for Short-Range Dispersion from a Continuous Ground-Level Source', *Boundary-Layer Meteorol.* **23**, 85–103.

Wilson, J. D., Thurtell, G. W. and Kidd, G. E.: 1981a, 'Numerical Simulation of Particle Trajectories in Inhomogeneous Turbulence II: Systems with Variable Velocity Scale', *Boundary-Layer Meteorol.* **21**, 423–441.

Wilson, J. D., Thurtell, G. W. and Kidd, G. E.: 1981b, 'Numerical Simulation of Particle Trajectories in Inhomogeneous Turbulence, III: Comparison of Predictions with Experimental Data for the Surface Layer', *Boundary-Layer Meteorol.* **21**, 443–463.

Wilson, J. D., Legg, B. J. and Thomson, D. J.: 1983, 'Calculation of Particle Trajectory in the Presence of a Gradient in Turbulent Velocity Variance', *Boundary-Layer Meteorol.* **27**, 163–169.