FOOTPRINT PREDICTION OF SCALAR FLUXES FROM ANALYTICAL SOLUTIONS OF THE DIFFUSION EQUATION

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Abstract. The use of analytical solutions of the diffusion equation for 'footprint prediction' is explored. Quantitative information about the 'footprint', i.e., the upwind area most likely to affect a downwind flux measurement at a given height z, is essential when flux measurements from different platforms, particularly airborne ones, are compared. Analytical predictions are evaluated against numerical Lagrangian trajectory simulations which are detailed in a companion paper (Leclerc and Thurtell, 1990). For neutral stability, the structurally simple solutions proposed by Gash (1986) are shown to be capable of satisfactory approximation to numerical simulations over a wide range of heights, zero displacements and roughness lengths. Until more sophisticated practical solutions become available, it is suggested that apparent limitations in the validity of some assumptions underlying the Gash solutions for the case of very large surface roughness (forests) and tentative application of the solutions to cases of small thermal instability be dealt with by semi-empirical adjustment of the ratio of horizontal wind to friction velocity. An upper limit of validity of these solutions for z has yet to be established.

1. Introduction

Any flux observation at an elevated point raises the question as to the effective upwind source area ('footprint') sensed by the observation, with 'source' understood to include negative flux densities. Every point- or area source will potentially contribute to the concentration or flux profile downwind to a degree that varies with distance from the source (x), elevation of observation (z), as well as with characteristics of the turbulent boundary layer and atmospheric stability. The question is particularly pertinent in the case of flux observations and flux mapping by aircraft; it may partly explain the lack of correlation between observed fluxes and underlying terrain (e.g. Durand *et al.*, 1987). Aircraft-based eddy correlation flux measurements have been made – apart from momentum and sensible heat – of ozone (Lenschow *et al.*, 1981 and 1982), water vapor (Grossmann and Bean, 1973; McBean and Peterson, 1975; Bean *et al.* 1976; Hacker, 1982; Schuepp *et al.*, 1987; Desjardins *et al.*, 1989) and CO_2 (Desjardins *et al.*, 1982 and 1989; Alvo *et al.*, 1984; Austin *et al.*, 1987). Fast response sensors are being developed to apply the technique to other trace gases, such as methane, and the use of such techniques is likely to grow due to their versatility of application, particularly in the interpretation of satellite observations at remote sites. With observations usually taken at flight levels of tens to hundreds of meters a quantitative estimate of effective source location becomes important. This paper will explore the use of analytical solutions of the diffusion equation for footprint prediction in a form that permits easy incorporation into analysis package of ground-based and airborne flux observation systems while a companion paper (Leclerc and Thurtell, 1990) will describe Lagrangian trajectory simulations that were used as a preliminary 'calibration' of such solutions.

A number of studies have addressed the problem of local advection, i.e., the relative contributions from localized sources at upwind distance x, for observation at point $(0, z)$, through analytical solutions of the diffusion equation. The review given below is not intended to be exhaustive and does not cover studies dealing primarily with the adjustment of the momentum boundary-layer downwind of a line of discontinuity in surfaces characteristics.

Philip (1959), Wilson (1982) and Horst and Slinn (1984) derived approximate analytical solutions to the two-dimensional diffusion equation for various idealized surface boundary conditions, relevant to downwind observations from the leading edge of infinitely wide crosswind area or line sources, assuming logarithmic or power laws for vertical velocity and diffusivity profiles. The Horst and Slinn solutions are among the very few that incorporate some effects of atmospheric stability. Wilson compared analytical solutions against predictions of a stochastic trajectory-simulation model and field observations on diffusion of SO_2 from the Prairie Grass Experiment, finding satisfactory agreement between analytical and numerical simulations and excellent agreement between numerical simulations and experimental data for neutral stability. None of these solutions are entirely straightforward in application, as discussed below.

The problem of downwind observation of two-dimensional upwind sources had originally been addressed by Pasquill (1972), based on analogy between momentum transfer and transfer of passive particles. For any height of observation (z), upwind ground-source regions are delineated from within which emissions are detected at a level exceeding an arbitrary threshold. Results are given for stable, neutral and unstable thermal stratification, based on very approximate numerical solutions of the two-dimensional diffusion equation, with an assumed constant stability- and roughness-independent crosswind spread of 30 degrees. Results showed isopleths expanding enormously as stable conditions are approached. The approach by Pasquill has been followed up by Schmid and Oke (1988) but details and results of simulations are not yet available. Again, these simulations are not simple to use and – as all such models – depend on assumptions about plume spread and stability effects whose validity has not yet been adequately tested.

A recent attempt to provide very simple approximate solutions for the case of source discontinuities of infinite crosswind extent by Gash (1986) is based on that of Pasquill (1972), as well as on earlier work by Sutton (1934) and Dyer (1963). However, the approximate solutions of the diffusion equation suggested by Calder (1952) were used. Advantages and disadvantages of this approach stem from its simplicity: No effort is made to satisfy an energy balance, neutral thermal stability is assumed and a uniform field for wind velocity (u) and turbulent diffusivity (K). Concentration and flux profiles can then be described approximately by exponential functions, with superposition in the case of a series of upwind discontinuities. Results were compared to the more rigorous but less easily applicable model of Dyer (1963), where $u(z)$ and $K(z)$ are represented by power functions; discrepancies were found to be $<20\%$ and often much smaller.

Barr and Kreitzberg (1975) used an entirely different approach, analogous to the diffusion of surface temperature variations into a semi-infinite medium. Boundary conditions are simple harmonic oscillations at the surface and zero amplitude at infinite distance. Their analysis is applicable to large scales, since u and stability-dependent K are also taken as constant with height. Solutions are exponentially damped (with wavenumber-dependent damping and phase lags relative to surface oscillation), permitting definition of heights and radii of influence for surface effects to be noticeable at the given point of observation.

Two-dimensional higher-order closure models have been applied to the problem of local advection by Rao *et al.*, (1974) and Rao (1975) for a transition from a smooth dry area to a wet, grassy one. The model consists of the usual set of conservation and transport equations and closure assumptions including gradient transport for higher moments. However, solutions are applicable only for downwind displacements of about 20 m. They show a small effect of surface roughness but a large effect of stability. Some fundamental limitations of higher-order closure in this context have been summarized by Wyngaard (1988).

The relative profusion of approximate analytical solutions coincides with scarcity of experimental data suitable for their verification. However, rapid recent advances in stochastic Lagrangian simulation of particle diffusion from ground sources of various spatial dimensions, such as through the Langevin equation, now promise some possibility of independent estimate, particularly since stochastic trajectory simulations can give good agreement with observed diffusion from line and area sources (Wilson, 1982), and with model experiments on diffusion in a water tank, wind tunnel and diffusion from ground sources in the field (de Baas *et al.*, 1986). They have also shown some success with prediction of diffusion from line sources in simple canopy situations (Leclerc *et al.*, 1988), albeit on a very small scale. Such simulations, reviewed in the companion paper (Leclerc and Thurtell, 1990), are based on ensemble-averaging of instantaneous point source releases. They are rapidly improving in physical realism and offer, perhaps, the most promising possibility for including realistic large-scale properties of turbulence in model predictions.

Given these facts, this paper explores the applicability of simple approximate solutions of the diffusion equation (primarily those proposed by Gash, 1986) to footprint prediction, since they lend themselves most easily to incorporation into analysis packages. Lagrangian trajectory simulations (themselves subject to simplifying assumptions, as detailed by Leclerc and Thurtell, 1990) will be used as a preliminary test to infer model usefulness. A tentative comparison of predictions against airborne concentration measurements in situations of local advection will also be presented.

2. Experimental Method

2.1. Stochastic (Langevin) simulation

Numerical simulations, against which analytical solutions are compared, are based on the Langevin equation. Time-averaged concentration profiles $c(x, z)$ were constructed from ensemble averaging of a large number of individual trajectories, at downwind positions x from an infinite cross-wind line source or, by superposition of line sources, from the leading edge of an infinite cross-wind area source. Flux profiles were obtained by gradient flux assumption. Details of the numerical computations, specific model assumptions and complete presentation of numerical results for a wide variety of spatial scales, surface characteristics and atmospheric stabilities are given by Leclerc and Thurtell (1990).

2.2. Airborne observations

Aircraft observations presented in this study were obtained during the airborne flux measurement program of the National Aeronautical Establishment (NAE) and Agriculture Canada in 1986. They are peripheral studies in situations of local advection, executed in addition to major study objectives over homogeneous terrain which have been published elsewhere (Schuepp *et al.*, 1987; Desjardins *et al.*, 1989). The Twin Otter research aircraft (MacPherson *et al.*, 1981) can be used for eddy-correlation flux measurements at heights down to 10 m, at airspeeds of 50 m s^{-1}. Apart from the three orthogonal components of turbulence, the aircraft measures (among other parameters) concentrations of passive admixtures (CO_2 and H_2O) with fast-response open-path infrared gas analyzers. Agreement between ground-based and airborne eddy correlation flux measurements over extended, homogeneous terrain, has been shown to be generally within 10% for CO_2, provided sampling run length is of the order of 15 km or more (Desjardins *et al.*, 1989), with larger discrepancies for H_2O and sensible heat due to more pronounced flux divergence in the vertical. The question of variability of airborne flux estimates has been addressed elsewhere (Wyngaard, 1983; Austin *et al.*, 1987; Schuepp *et al.*, 1989).

The flight program under discussion included six trajectories of 17 km length across Flatland Island (49° 44′ N, 88° 19′ W) in Lake Nipigon, approximately 2.2 km × 3.5 km in dimension, with average elevation of 50 m. The trajectory crossed the island at an angle of about 20° to the minor axis, over a distance of 2.4 km, in the direction of prevailing wind, with mean upwind and downwind sections beyond the island of about 5.9 km and 8.8 km respectively. Flight altitude was 100 m above the lake and approximately 50 m over the island. Atmospheric conditions were slightly unstable during these flights (average $z/L \approx -0.2$, with L the Monin–Obukhov length). Flux estimates were high-pass filtered at 0.03 Hz, i.e., at wavelength components of about 1600 m.

3. Analyses and Discussion

3.1. Review of some analytical solutions

Although the emphasis of the present study lies in footprint analysis of flux profiles, analytical soutions will initially be reviewed in terms of their prediction of concentration profiles. This is justified by the fact that flux profiles are calculated from concentration profiles through a gradient-flux assumption. Also, it may be easier, in some situations of limited sampling length for airborne observations, to use the concentration field, rather than the flux field, as a confirmation of general validity.

Considering an infinite cross-wind area source of uniform vertical flux density, satisfying the flux boundary condition of 0 for $x < 0$ (outside the source area) and Q_0 for $x \geq 0$, i.e., an 'active' area preceeded upwind by an inactive one, the vertical concentration profile $c_x(z)$ at downwind distance x from the leading edge is calculated as follows for neutral stability:

(a) Philip (1959) expressed concentration (for $Q_0 = 1$) as $c(\eta, \beta)$, where η is a compound variable, combining x and z as follows:

$$\eta = \eta(x, z) = \frac{u_1 z^{2+m-n}}{(2+m-n)^2 K_1 x}, \tag{1}$$

u_1 and K_1 are defined by the conjugate power law for wind and diffusivity of $u(z) = u_1 z^m$ and $K = K_1 z^n$. With β defined as $(2+m-n)/(1-n)$, the concentration is then expressed in terms of the surface concentration c_0 of the active region as

$$c(\eta, \beta) = c_0\left[1 - \Gamma\left(1 - \frac{1}{\beta}\right)\eta^{1/\beta} + \sum_{k=1}^{\infty} \frac{(-1)^{k+1} k}{k!(k\beta - 1)}\right], \tag{2}$$

where m and n (as given by Philip) might be 1/7 and 6/7, respectively, i.e., $\beta = 9$ and $\Gamma(1 - 1/\beta) \cong 1.076$.

The series in Equation (2) is absolutely convergent for all finite η. However, convergence for $\eta > 2$ becomes very slow, with round-off errors affecting the result in normal computational procedures. For this reason the value for $\eta = 4$ is listed (by Philip) as 'dubious'. For larger values of η, an asymptotic expansion is presented which also requires a large number of terms for convergence, with unacceptable round-off error at values close to 4, making its use impractical in that range.

With the values of m, n, u_1 and K_1 suggested by Philip, the value of $\eta =$ 4, where neither Equation (2) nor the asymptotic expansion shows practical convergence, corresponds to downwind displacements of a few hundred to 1000 m for heights of 20 to 50 m. This is precisely the range of interest for airborne observations. For this reason the Philip solutions, in spite of their demonstrated advantages at smaller scales, are not used in the subsequent analysis.

(b) Wilson (1982) solved the transformed two-dimensional diffusion equation by an approximation suggested by Shwetz (1949), retaining the first two terms. A logarithmic profile is used for $u(z)$ and concentration is expressed in terms of a partitioning factor r, characterizing the relative contributions from each retained term and a function $\delta = \ln(z_\delta/z_0)$, with z_δ the upper edge of the plume of emitted material and z_0 the roughness length. For neutral stability, r may be approximated by 0.5, but the definition of δ is implicit, requiring solution by successive approximation. For this reason these solutions are not easily integrated into application-oriented analysis packages.

(c) Horst and Slinn (1984) expressed the concentration profile at downwind distance x by the convolution

$$c_x(z) = \int_0^x F(\xi) D(x - \xi, z)\, \mathrm{d}\xi\,, \tag{3}$$

with $F(\xi)$ the flux density at the ground, at position ξ, and D a fairly complex expression of coordinates (x, z) which can be reduced, for the case of a mixing length assumption for $K(z)$ and a logarithmic profile for $u(z)$, to

$$D(x, z) = \left[\frac{A}{\bar{z}(x) u(c\bar{z})}\right] \mathrm{e}^{-(z/b\bar{z})^s}\,, \tag{4}$$

where $\bar{z}$ is the mean height of the plume of emitted material at downwind distance x, obtained from $(\mathrm{d}\bar{z}/\mathrm{d}x) = K(q\bar{z})/(q\bar{z}u(q\bar{z}))$ (Van Ulden, 1978). A, b, c and q are constants that depend on the parameter s, which varies from ≈ 1 for unstable conditions to ≈ 2 for stable stratification. These solutions can be adapted to unstable conditions through adjustment of s (and through it of constants A, b, c and q) and by applying the usual stability corrections to velocity and K-profiles, but the inclusion of these ill-defined constants makes their practical application unattractive.

(d) Gash (1986) proposed the use of the approximate solutions given by Calder (1952) for neutral stability, which give the concentration at point $(0, z)$ resulting from an infinite crosswind line source located at an upwind distance x in a uniform windfield (U and K constant), as

$$\rho(x, z) = \frac{Q_L}{k u_* x}\, \mathrm{e}^{-Uz/ku_*x}\,, \tag{5}$$

Q_L is source strength per unit length, k the von Karman constant, u_* the friction velocity, z the height above the zero displacement (d), and U the assumed constant windspeed, defined as the average windspeed between the surface and observation height z. Assuming a logarithmic profile for $u(z)$, with z representing observation height above the ground, U is given by

$$U = \int_{d+z_0}^{z} u(z)\,\mathrm{d}z \Big/ \int_{d+z_0}^{z} \mathrm{d}z = \frac{u_*[\ln((z-d)/z_0) - 1 + z_0/(z-d)]}{k(1 - z_0/(z-d))} \tag{6}$$

Equation (6) is equivalent to the (corrected) Equation (11) of Gash (1986).

The vertical concentration profile at downwind distance x from the leading edge of our hypothetical 'active' area is then obtained by integrating over all upwind line sources between 0 and x as

$$c_x(z) = \frac{Q_0}{ku_*} \int_0^x \frac{1}{x} \mathrm{e}^{-U(z-d)/ku_*x}\,\mathrm{d}x\,, \tag{7}$$

where Q_0 is the area flux density. Since the integrand is indeterminate at $x = 0$, this integral can only be evaluated approximately, by numerical integration starting from a small value $x \neq 0$. However, the vertical gradient of concentration, as the derivative of the integral and hence the integral of the derivative, is well behaved and equal to

$$\frac{\mathrm{d}c_x(z)}{\mathrm{d}z} = -\frac{Q_0}{ku_*(z-d)} \mathrm{e}^{-U(z-d)/ku_*x}\Big|_0^x = -\frac{Q_0}{ku_*(z-d)} \mathrm{e}^{-U(z-d)/ku_*x} \tag{8}$$

This permits easy estimation of flux profiles under a simple mixing-length assumption of $F(z) = K(\mathrm{d}c/\mathrm{d}z) = ku_*(z-d)(\mathrm{d}c/\mathrm{d}z)$.

Similarly, the relative contribution to the vertical flux at height z, stemming from an infinite crosswind source of unit width at an upwind distance x, is obtained simply by the derivative of the concentration as given by Equation (5), multiplied by $ku_*(z-d)$, i.e., by

$$\frac{ku_*(z-d)(\mathrm{d}\rho/\mathrm{d}z)}{Q_0} = \frac{1}{Q_0}\frac{\mathrm{d}Q}{\mathrm{d}x} = (-)\frac{U(z-d)}{u_*kx^2} \mathrm{e}^{-U(z-d)/ku_*x}\,. \tag{9}$$

The relative-flux-density designation of $(1/Q_0)\,\mathrm{d}Q/\mathrm{d}x$ underlines the fact that integration of the right hand side expression in Equation (9), or the summation of $\mathrm{d}Q/Q_0$ from $x = 0$ to infinity, is unity, i.e., the total relative flux density at the observation point. Equation (9) thus defines the one-dimensional '*footprint*', the relative importance of sources at upwind distances x to the flux measurement at point (x, z). Thus, the position of the peak of the footprint (x_{max}), i.e. the area to which the observation at $(0, z)$ is most sensitive, can be estimated from the vanishing derivative of the footprint function with respect to x as

$$x_{\mathrm{max}} = \frac{U}{u_*}\frac{(z-d)}{2k}\,. \tag{10}$$

Introducing x_{max} into Equation (9), the maximum relative contribution to the flux 'signature' at the observation point (peak of the footprint function) would then be

$$\left(\frac{1}{Q_0}\frac{dQ}{dx}\right)_{max} = \frac{4u_*k}{u(z-d)}\,e^{-2}\,. \tag{11}$$

The obvious advantage of these solutions lies in their 'mechanical simplicity', resulting from the simplified assumptions about the wind field. For example, vertical flux profiles for a sequence of n crosswind strips upwind of the observation point at $x = x_0$, with strip flux densities Q_i bordered at the upwind side at displacements x_i (as measured from x_0), would be calculated according to Equation (8) as

$$F(z) = -\sum_{i=1}^{n} Q_i\, e^{-U(z-d)/(ku_*x)}\Big|_{x_{i-1}}^{x_i}\,. \tag{12}$$

3.2. Concentration Profiles

Concentration profiles given for neutral stability by Wilson (1982) and Horst and Slinn (1984) are compared in Figure 1 with those calculated from the solutions of Gash (1986) for downwind displacements of 20 m and 100 m. The numerical integration in Equation (7) was initiated at $x = 0.01$ m (instead of $x = 0$) to avoid the indeterminate value of the integrand as previously discussed. Estimates are stable, i.e., changes in step size or point of initiation do not affect the result within measurable accuracy. Concentration is expressed nondimensionally as (cu_*/kQ). The assumed roughness length of 0.5 cm, equal to the one used by Horst and Slinn (1984), gives a U/u_* ratio of 12.5 at a height of 2 m (Equation (6)). While this value of z_0 would be small for grassland, the resulting U/u_* ratio corresponds approximately to the value of 12 deduced, e.g., from wind profile measurements by Ripley and Redman (1975) for a height of 2 m above prairie grass surface cover and neutral stability, at windspeeds of about 3 m/s.

Figure 1 shows close agreement between the Wilson and Horst–Slinn solutions, and very approximate agreement between them and the Gash profiles for heights above 0.5 to 1 m, in terms of general magnitude, slope and relative differences between downwind displacements of 20 and 100 m. The discrepancy in profile curvature reflects a weakness in the assumption underlying Equation (6) that a diffusing particle would, on the average, experience the average windspeed between the ground and the observation level. This weakness could be corrected by adjustment of the U/u_* ratio, but the associated empiricism, in absence of a satisfactory analytical framework, is not attractive. In the present context, we conclude that profiles predicted by Equation (7), with U/u_* ratios given by Equation (6), may be capable of first-order approximation to more sophisticated analytical solutions. But their limitations close to the ground, and possibly also at upper heights where absolute concentration becomes small, must be kept in mind.

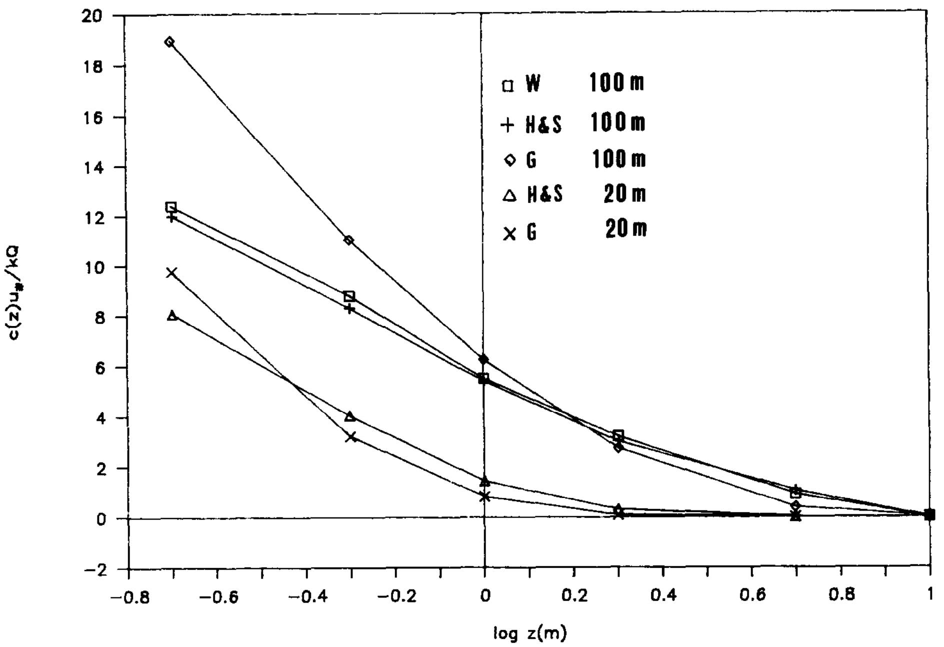

Fig. 1. Nondimensional concentration profiles with height (z), 20 m and 100 m downwind from the leading edge of an infinitely-wide area source. Shown are predictions by Wilson (1982) (W), Horst and Slinn (1984) (H&S) and Gash (1986) (G).

3.3. Footprint Prediction

Within the limitations expressed above, we may construct the 'footprint', i.e., the fractional flux from upwind areas x (as measured from the point of observation) for various observation heights z, by plotting the function $(1/Q_0)\,dQ/dx$ in Equation (9). These analytical predictions can then be compared against the numerical (Langevin) simulations of Leclerc and Thurtell (1990). Figure 2 shows results for observation heights (z) of 21, 41 and 75 m above a tall grass or small crop surface with $d = 0.3$ m, $z_0 = 0.06$ m under neutral conditions, with U/u_* ratios calculated from Equation (6). The numerical simulations assumed $u_* = 0.4$ m s^{-1} and a source height of 0.5 m.

Figure 2 shows the striking dependence of 'area of influence' on measuring height, with an observation at 20 m primarily affected by sources at an upwind distance of 300 to 400 m, increasing to almost 2 km for a height of 75 m. Agreement between analytical and numerical predictions is good for the 21 m observation height, with some systematic difference observable at heights of 41 and 75 m. The difference can be effectively reduced (dashed lines in Figure 2), if the flow velocity at the given height z, rather than the average velocity U between z and the ground, is used, i.e., with U/u_* in Equation (9) given by $u(z)/u_* = k^{-1}\ln((z-d)/z_0)$ rather than by Equation (6).

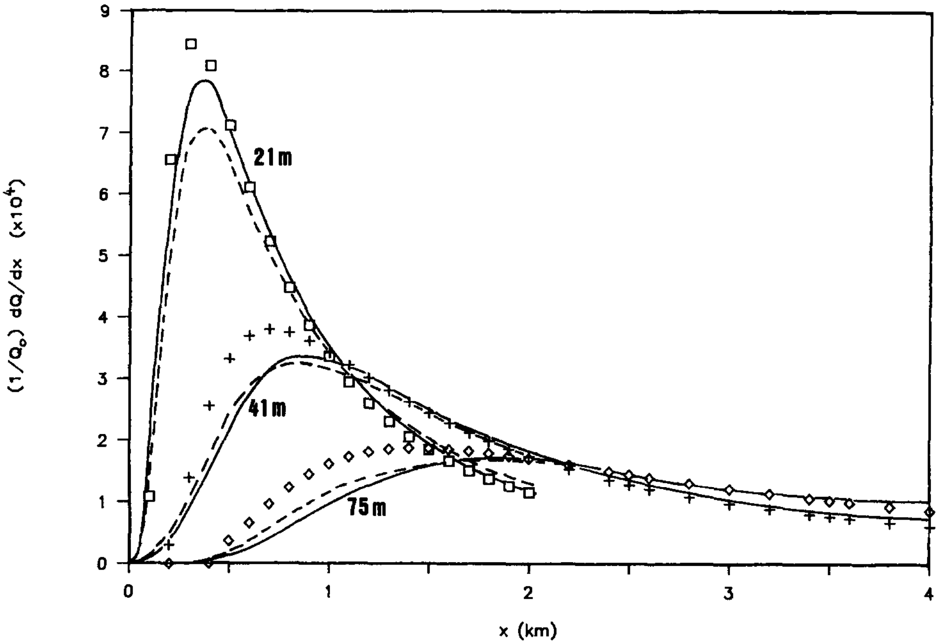

Fig. 2. Footprint predictions from Equations (9) and (6) (symbols) and numerical predictions by Leclerc and Thurtell (1990) (lines) for observation heights of 21, 41 and 75 m, with $d = 0.3$ m and $z_0 = 0.06$ m. Dashed lines are results for U/u_* based on local, rather than average, windspeed.

While heights of 21 to 75 m are of interest to airborne observations, lower heights should be considered due to their potential application to tower data. Figure 3 shows a comparison between the predicted footprint and numerical simulations for heights of 3, 5 and 9 m. Overall, estimates based on Equations (9) and (6) give reasonable agreement (within about 20%) with numerical simulations, down to heights of 1 m (not shown, but easily verified by comparing analytical predictions with the graphical results presented by Leclerc and Thurtell, 1990). Again, the agreement between analytical and numerical predictions could be improved by empirical adjustment of the U/u_* ratio. Since U, as defined by Equation (6), is less than $u(z)$ at any level z, a best-fit reduction factor (RF) for U relative to u can be determined for optimum agreement in peak position between numerical and analytical predictions. Between heights of 1 and 40 m, RF was found to be linearly correlated with $b = \ln((z - d)/z_0)$ and the regression line of $\mathrm{RF} = 0.204 + 0.128b$ had a correlation coefficient of 0.97 and standard error of 0.054. The resulting adjusted footprint predictions are shown by dashed lines in Figure 3. This means that for optimum footprint agreement with numerical simulations, U should be 0.51 and 0.94 of the local horizontal windspeed u at heights of 1 m and 20 m, respectively, while Equation (6) suggests factors of 0.66 and 0.83, respectively, for the same heights. It is understood the parameters of

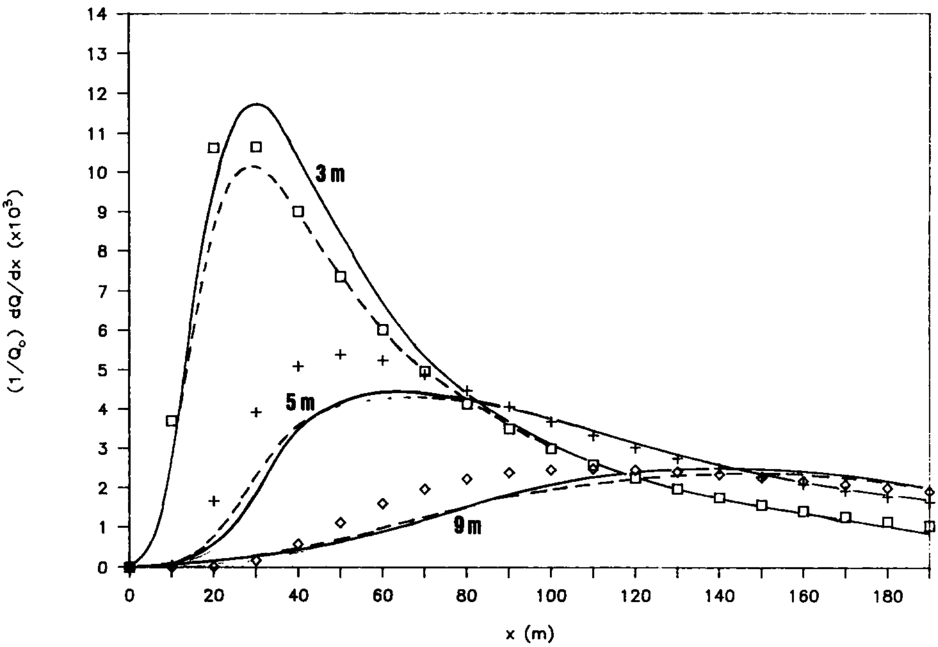

Fig. 3. Footprint predictions from Equations (9) and (6) (symbols) and numerical predictions (lines) for observation heights of 3, 5 and 9 m, with $d = 0.3$ m and $z_0 = 0.065$ m. Dashed lines correspond to adjusted U/u_* ratios as described in the text.

the regression equation given above are likely to be different for different surface characteristics. Keeping in mind the undesirability of empirical adjustment factors, the limitations of the numerical simulations, and realistic expectancies of accuracy in most micrometeorological modeling, we might conclude from Figures 2 and 3 that the predictions of Equations (9) and (6) give adequate footprint representation for heights between 1 and 20 m, with a suggestion that local, rather than average, windspeed be used for heights above that level.

For smoother surfaces (with d of the order of several cm) the footprint expands: numerically simulated positions $x_{\max}$ increased by factors of about 1.37 and 1.63 for observation heights of 9 and 19 m, respectively, when d was decreased from 0.3 m (with $z_0 = 0.06$ m) to 0.066 m (with $z_0 = 0.013$ m), while Equation (10) predicts a corresponding increase of 1.3 and 1.36. As a very first approximation, and within the uncertainty of the numerical simulations, this may be considered as an indication that Equation (10) possesses the right order of sensitivity for shifts in footprint peak with roughness changes relevant to grasslands or small crops.

In Figure 4, numerical footprint simulations and predictions from Equation (9) are compared for the case of a forest canopy at heights of 25, 41 and 79 m, assuming a zero-displacement of 12 m, roughness length of 2.6 m, source height of 16 m and u_* (for numerical simulations) of 0.4 m s^{-1}. As a first approximation,

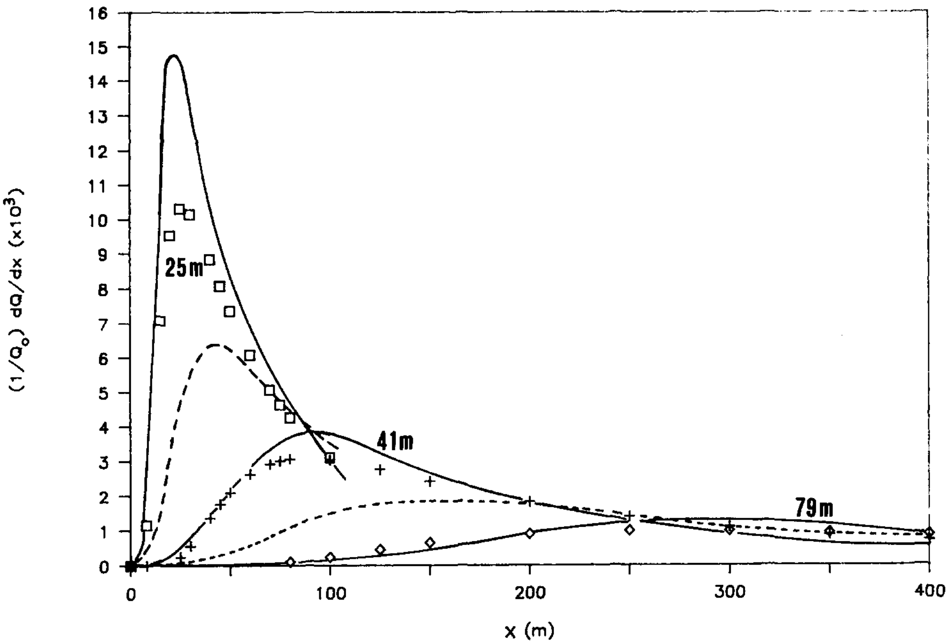

Fig. 4. Footprint predictions from Equation (9), with $U/u_* = 0.4u(z)/u_*$ (symbols), and numerical predictions (lines) for observation heights of 21, 41 and 79 m above a forest canopy, with $d = 12$ m and $z_0 = 2.6$ m. Dashed and dotted lines give results for U/u_* based on Equation (6) for 25 and 41 m, respectively.

acceptable agreement is obtained for all three heights z when U/u_* ratios are taken as 0.4 of $u(z)/u_*$, while U/u_* ratios derived from Equation (6) are equivalent to 0.64 to 0.73 of $u(z)/u_*$ for the given range of z. Predictions based on the latter are also shown in Figure 4 (dashed and dotted lines); the pronounced difference between them and the numerical simulations most likely reflects once more some inadequacy of defining the constant windspeed for Calder's solution by the average windspeed between $d + z_0$ and z. Comparison with Figure 2 illustrates the 'shrinking footprint' of the rough surface.

3.4. Cumulative Footprint Prediction (Effective Fetch)

In terms of the Gash solutions, the cumulative normalized contribution to the flux measurement (CNF) at height z, from an upwind area bounded by a distance x_L from the point of observation, is obtained by integration of Equation (9). For neutral stability it is

$$\mathrm{CNF}(x_L) = (-) \int_0^{x_L} \frac{U(z-d)}{u_* k x^2} \mathrm{e}^{-U(z-d)/ku_* x} \, \mathrm{d}x = \mathrm{e}^{-U(z-d)/ku_* x_L} . \tag{13}$$

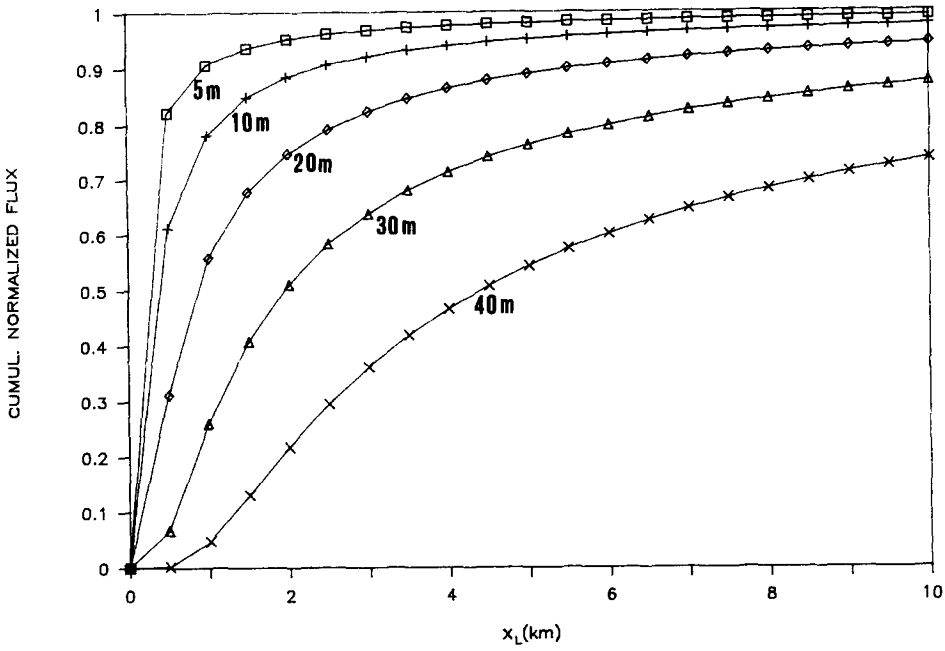

Fig. 5. Cumulative normalized flux as a function of upwind distance, for selected observation heights from 5 to 80 m, with $d = 0.3$ m and $z_0 = 0.06$ m.

Figure 5 shows plots of CNF(x_L) for heights of 5, 10, 20, 40 and 80 m, for the case of $d = 0.3$ m and $z_0 = 0.06$ m, with U/u_* ratios derived from Equation (6).The results indicate, e.g., that >80% of the measured flux at a height of 5 m can be expected to come from within the nearest 500 m of upwind area, but only about 30% at an observation height of 20 m.

3.5. Effects of Atmospheric Instability

Numerically-predicted effects of atmospheric stability on footprints are presented for various degrees of surface roughness by Leclerc and Thurtell (1990). Only a very preliminary analysis on its possible representation within the given analytical solutions will be attempted here since the focus of this paper is on solutions that have been formulated for neutral conditions.

Within expected reliability and given range of experimental parameters, the numerical simulations suggests a significant effect of instability on footprint location and intensity, as soon as z/L falls below about -0.2, with footprints contracting under effects of increasing instability. If we ask to what degree the analytical solutions used above might be modified to reflect such changes, we might speculate that the U/u_* ratio is the most likely place to apply a correction, since momentum stability corrections account for changes in wind profile shape relative to that in neutral condition. If we multiply the U/u_* ratios in Equation

(9) by a momentum stability correction function (ϕ_m), in analogy to stability corrections applied in Monin–Obukhov scaling, the peak footprint location (x_{max}, Equation (10)) would be reduced by the function ϕ_m. Using, for the sake of this exercise, a correction function for momentum transfer of $\phi_m = (1 - 16(z - d)/L)^{-1/4}$ (Dyer, 1974), the shifts in peak footprint position would range from 0.90 to 0.74, for heights between 9 and 39 m, for surface roughnesses with d between 5 and 30 cm in a transition from neutral condition to $L = -320$ m. For a transition from neutral to $L = -40$ m, the shift would range from 0.66 to 0.47 for the same heights. These estimates are somewhat more pronounced, but of the same order, as the numerically predicted ones (Leclerc and Thurtell, 1990) of 0.96 to 0.84 and 0.7 to 0.55, respectively. For forest canopies, the shifts estimated on the basis of Equation (10), with the applied stability correction, should range from 0.73 to 0.51 for heights between 25 and 79 m, in a transition from neutral to $L = -80$ m, very close to the numerically-predicted shifts of 0.7 to 0.57.

These very preliminary studies point out the need for practically useful analytical solutions which specifically include the effect of stability, perhaps based on the approach of Horst and Slinn (1984); they also underline the need for experimental tests of predictions.

3.6. Aircraft Observation

Given the series of repeated flight trajectories over Flatland island (section 2) it may be of interest to compare the downwind flux signature for CO_2 predicted by analytical solutions with observed flux measurements. Agreement cannot be expected a priori due to the significant change in surface roughness involved along the trajectory.

Figure 6 shows average flux estimates for the six run segments (two segments upwind and three downwind of the island), with standard deviations of estimates. The standard deviation of the island flux estimate is 32%, i.e., similar to that observed over homogeneous terrain for sets of comparable run length (Schuepp *et al.*, 1989) and approximately 50% lower than those expected on the basis of the analysis by Wyngaard (1983), most likely due to the fact that measured fluxes were based on high-pass filtered data. No attempt was made to estimate local flux variations within segments due to the rapidly increasing variability of flux estimates over shorter sampling distances. Also included in Figure 6 are calculated flux profiles, along the flight trajectory, based on the analytical solutions of Gash (1986) and Barr and Kreitzberg (1975) for heights of 50 m. The Gash solutions are defined by Equations (8) and (12); if x is the downwind displacement from the leading edge of the island, the horizontal profile of vertical flux $F_z(x)$ is given by

$$F_z(x) = Q_{isl}[e^{-U(z-d)/ku_*x}] \text{ for } x \text{ within the island, and by}$$

$$F_z(x) = Q_{isl}[e^{-U(z-d)/ku_*x} - e^{-U(z-d)/ku_*(x-2400)}], \qquad (14)$$

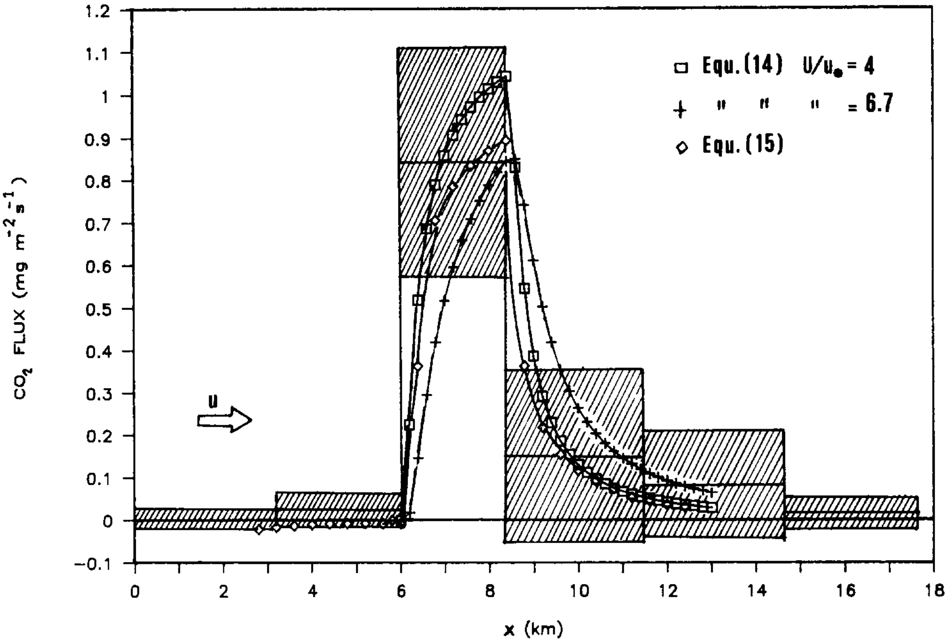

Fig. 6. Flux measurements from aircraft for six segments along cross-island trajectories: mean values and range equivalent to standard deviation (shaded areas). Symbols indicate results of flux predictions from analytical solutions by Gash (1986) (Equation (14)) and by Barr and Kreitzberg (1975) (Equation (15)).

for x downwind of the island. Q_{isl} is the average surface CO_2 flux density of the island, taken as $1.2\,\text{mg}\,\text{m}^{-2}\,\text{s}^{-1}$ from an approximate extrapolation of the aircraft observations. Gash solutions are presented for the case of $U/u_*=6.7$, corresponding to $0.4\,u(z)/u_*$ at $z=50$ m, for a logarithmic profile with $d=12$ m and $z_0=2.6$ m, which was found to give satisfactory agreement with numerical footprint prediction over extended forests (section 3.3) and, arbitrarily, for a further reduced $U/u_*=4$.

The Barr and Kreitzberg (1975) analysis gives solutions for simple harmonic variation in horizontal surface flux profiles. These solutions were incorporated into the Fourier transform of a rectangular pulse of width 2400 m with height of Q_{isl}, so that the real part of the solution is then represented by the integral (over wavenumber k) as

$$F(x, z) = Q_{\text{isl}} \int_0^{\infty} \frac{2}{\pi k} \sin(kL)\, e^{-\sqrt{uk/2Kz}} \cos k\left(\frac{zu}{\sqrt{2Kuk}}\right) dk\,, \tag{15}$$

where K is the turbulent diffusivity (taken as $10\,\text{m}^2\,\text{s}^{-1}$) and L the half-width of the pulse (1200 m, with the pulse assumed to be centered on $x=0$ for the transform). Windspeed was taken as $2.5\,\text{m}\,\text{s}^{-1}$, in accordance with aircraft data. The numerical integration (Simpson's rule) over wavenumber (k) to infinity was approximated by 80 steps of size 0.5, with all lengths normalized to L, i.e., up to a maximum k-value of 40 or a minimum wavelength component of $(2\pi)/40$ units of L (about 188 m).

Figure 6 shows overall agreement, in trends and absolute values, between airborne flux estimates and analytical solutions and between the two analytical solutions considered. While the aircraft data from the given flight paths could not be expected to give, with any degree of reliability, the local variation of flux estimates across the local advection zone of the island, one might hypothesize that the given analytical solutions can provide a reasonable representation of such variations. The given data base and experimental conditions are not adequate to evaluate the respective merits of the two solutions as far as differences between their predictions are concerned, but the operational advantage of prediction by Equation (14) as compared to the approximate numerical solution of Equation (15) is evident.

4. Summary and Conclusions

This paper attempts to fit some existing simple analytical solutions to numerical simulations of flux profiles in situations of local advection and – in one case – compares analytical predictions against aircraft-based flux measurements over an isolated island. There exists no a priori justification for using solutions which were derived, for example, for uniform wind and diffusivity fields in situations where such assumptions are clearly unrealistic. But there exists a pressing need for manageable analytical expressions capable of giving order-of-magnitude predictions of upwind areas most likely to affect a point measurement at a given height. Numerical predictions of atmospheric diffusion in situations of local advection are rapidly becoming more realistic but they are time-consuming in execution and cannot easily be incorporated into real-time operational observation packages.

The analyses presented here can only be considered a first step. The implicit assumption that the numerical simulations are 'correct' and form a suitable basis for 'calibration' of analytical solutions may be challenged. Such simulations also contain important simplifying assumptions (Leclerc and Thurtell, 1990) and have yet to exploit fully their potential for realistic representation of the surface boundary layer, with its complement of mechanical and convective turbulence. Numerical predictions depend strongly on surface roughness which, in our analysis, is represented by the conventional parameters of zero displacements and roughness length. The determination of such parameters, for realistic surface vegetation and changing wind conditions, is not easy.

However, within the limitations of our analysis it appears that existing analytical solutions can give satisfactory agreement with numerical simulations and the limited aircraft data presented above. The emphasis of this paper is on the solutions proposed by Gash (1986) which, due to their structural simplicity, can be easily applied under operational conditions. General agreement between analytical simulations and numerical simulations, in terms of spatial distribution and absolute magnitude, could be obtained by appropriate choice of the U/u_* ratio which dominates the Gash solutions. Insofar as turbulent diffusion scales with z_0, it should be possible to express the relationship between U and u_* in a dimensionless form when heights are expressed in units of z_0. Gash did this in a form equivalent to our Equation (6) which appears to give satisfactory results for a wide range of combinations of z, d and z_0 given in this paper. Exceptions, as in the case of large surface roughness (forest), are most likely attributable to inadequacy of the underlying assumption that the constant windspeed required for the Calder solutions, i.e., the average windspeed experienced by a diffusing particle, equals the average windspeed U between the ground (z_0 above the zero-placement) and observation height z.

An upper limit for observation heights where these solutions are applicable has yet to be determined, preferably by a program of airborne flux measurements parallel to – and at varying distances from – an 'infinite' straight line of discontinuity in surface flux. Deviations from the given solutions, both numerical and analytical, must be expected at heights where convective effects start to dominate over surface-generated mechanical turbulence. Such findings would be strongly dependent on the degree of atmospheric instability. Work is also needed on the case of spatial discontinuities in surface roughness and buoyancy effects (Bowen ratio).

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