Abstract
We revisit the data from Project Prairie Grass to explore some fundamental aspects of vertical dispersion in the atmospheric surface layer using modern stochastic theories of turbulent dispersion. In particular, we examine the relationship between the diffusion equation (K-theory) and first-order Lagrangian stochastic models (Langevin models) over a range of stabilities. We also attempt to resolve some conflicting earlier studies that imply significantly different values for the von Karman constant for the transfer of matter, or equivalently of the turbulent Schmidt number. Finally, we assess the importance of surface deposition in the Project Prairie Grass data.

Introduction
Project Prairie Grass is the name given to a dispersion experiment carried out in the atmospheric boundary layer near O’Neill, Nebraska in the summer of 1956. During the experiment nearly 70 releases of SO₂, each of 10 minutes duration, were sampled at a height of 1.5 m on arcs up to 800 m downwind of the source. In addition, vertical profiles were measured 100 m downwind of the source. The dispersion experiments were supported by micro-meteorological data including wind, temperature and humidity profiles. Project Prairie Grass remains one of the most comprehensive atmospheric dispersion experiments ever conducted.

The Project Prairie Grass (PPG) data set [1] has been widely used to test and assess theories of vertical turbulent dispersion in the atmospheric surface layer. Our interest here is in Lagrangian stochastic modelling, so we review briefly work with this focus, including that based on solution of the diffusion equation. Our main concern is to resolve some apparent conflicts, especially regarding the magnitude of the effective vertical diffusivity, and the implications this has for the value of the more fundamental Lagrangian structure function constant C₀ which is central to modern Lagrangian stochastic modelling. All the studies of interest here, and the present work, deal with the crosswind integrated concentration from a point source.

Previous Work
Nieuwstadt and van Ulden [11] solved the 1-D diffusion equation with vertical diffusivity K equal either to the vertical diffusivity for heat Kυ or to 1.35Kυ, where Kυ is the diffusivity for momentum. They used Kansas forms [2] for the wind profile and for the diffusivities and compared theoretical and experimental estimates for the centre-of-mass \( \mathcal{E} \) of 22 vertical profiles of the concentration at a distance 100 m downwind of the source.

In stable, neutral and moderately unstable conditions they concluded that predictions using both forms of the diffusivity agree well with the observed values of \( \mathcal{E} \). Under strongly unstable conditions, there is a large difference between the two alternative diffusivities and the data lie between the two. They questioned the use of the diffusion equation under these conditions.

Gryning et al. [6] extended Nieuwstadt and van Ulden’s results to include comparisons with the shape factor s and with the concentration at a height of 1.5 m. They also explored the influence of dry deposition, concluding that it improved comparisons with the data.

Various authors have compared the predictions of 1-D and 2-D Langevin equations with the PPG data [14]. For near-neutral conditions Wilson et al. [18] and Davis [3] found that good agreement with the data is obtained using a von Karman constant \( \kappa_{max} \approx 0.4 \), and with an enhanced von Karman constant for matter \( \kappa_{max} \approx 0.63 \), which according to Davis “allows for a little loss of SO₂ at the surface through dry deposition”. Reid [13] found a similar result in comparisons with data from Porton experiments. On the other hand, Ley [8] obtained a good fit to a profile based on representative values of \( \mathcal{E} \) and s derived by Nieuwstadt and van Ulden using \( \kappa_{max} = \kappa_{vmax} = 0.41 \).

Under diabatic conditions, Wilson et al. [18] used \( \kappa_{max} \approx 0.63 \) and effectively tuned the stability corrections to the diffusivity, obtaining good agreement with the observations for individual runs. Ley and Thomson [9] averaged measured profiles with similar values of Obukhov length L and, using \( \kappa_{max} \approx 0.41 \) and standard stability corrections, obtained good agreement with these profiles except close to the ground where the size of their time step caused an under-estimation of the concentration.

More recently, Venkatram and Du [17] and Du and Venkatram [4] used 1-D and 2-D Langevin models respectively in comparisons with the crosswind integrated concentration at a height of 1.5 m. Their approach differs from the earlier work described above, but corresponds roughly to \( \kappa_{max} \approx 0.65 \) for the 1-D model and \( \kappa_{max} \approx 0.92 \) for the 2-D model.

We can summarise the issues and apparent conflicts arising from these studies as follows:
1. How good an approximation is the diffusion equation? Some studies using the diffusion equation, with or without deposition, show agreement with the data.
2. What is the value for \( \kappa_{max} \)? Different Langevin model studies have claimed good agreement with the PPG data using significantly different values.
3. What is the role of deposition? Some studies claim it improves agreement with the observations, while others suggest it is not important or ignore it.

Theory
Nieuwstadt and van Ulden [11] and Gryning et al. [6] solved the 1-D diffusion equation. Here we have reproduced their results using a stochastic differential equation version of the 1-D diffusion equation. Our model equations are

\[
\begin{align*}
\frac{dz}{dt} &= \frac{\partial K}{\partial z} dt + \sqrt{2K} dz \\
u &= U(z) \\
\frac{dx}{dt} &= u dt,
\end{align*}
\]

(1)
where \( u \) is the streamwise velocity, \( x \) and \( z \) are the streamwise and vertical displacements along a fluid trajectory and

\[
K = \kappa_{\text{ref}} u \cdot z / \theta_{\text{ref}}
\]  

(2)
is the diffusivity. We use the Kansas forms [2] for the dimensionless temperature gradient \( \theta_{\text{ref}} \) and the mean wind speed \( U \), with a von Karman constant \( \kappa_{\text{ref}} \approx 0.35 \). Note though, we allow the von Karman constant for matter to vary from this value.

We also use a 2-D Langevin equation that can be represented by stochastic differential equations of the form [4]

\[
dw = \frac{C_{\xi \varepsilon}}{2} \left[ \lambda_{w+w} + \lambda_{w-w} \right] dt + \frac{\sqrt{2}}{2} \left( 1 + \lambda_{w+w} + \lambda_{w-w} \right) \sigma_{w} \frac{\partial}{\partial z} w dt + \sqrt{C_{\xi \varepsilon}} \sigma_{\xi} d\xi
\]

\[
du' = -\frac{C_{\xi \varepsilon}}{2} \left[ \lambda_{u'^{+}} + \lambda_{u'^{-}} \right] dt + \sqrt{C_{\xi \varepsilon}} \sigma_{\xi} d\xi
\]

\[
u = u' + U(z)
\]

\[
\Delta = \frac{\sigma_{w}^2}{\sigma_\varepsilon}
\]

(3)

and the streamwise velocity fluctuations are given by

\[
\sigma_\varepsilon = 2.5 \mu_\varepsilon.
\]

Here, \( \mu_\varepsilon \) is the friction velocity and \( L \) is the Monin-Obukhov length. In (3) \( C_{\xi \varepsilon} \) is formally equal to the constant in the inertial subrange of the Lagrangian velocity structure function, \( \varepsilon \) is the rate of dissipation of turbulence kinetic energy and \( \lambda_{\text{eff}} \) is a component of the inverse Reynolds stress tensor. In both (1) and (3) \( \sigma_{\xi}^2 \) is the increments Wiener process [5].

We determine the product \( C_{\xi \varepsilon} \) by matching the vertical component of the diffusion limit of the Langevin equation to (1) with the diffusivity given by (2). Thus we have

\[
C_{\xi \varepsilon} = 2 \left( \sigma_\varepsilon^2 + u'^2 \right) / K.
\]

(6)

This is equivalent to prescribing a Lagrangian time scale by

\[
T_i = \frac{2 \sigma_{\xi}^2 \sigma_{w}^2}{C_{\xi \varepsilon}} = \frac{\sigma_{\xi}^2}{\sigma_{\varepsilon}^2 + u'^2} K.
\]

(7)

The stochastic differential equations are solved numerically by generating trajectories with initial conditions \( z = z_i, x = 0 \) and, for (3), initial random velocities drawn from a 2-D Gaussian distribution with mean \( U \), variances \( \sigma_{\xi}^2 \) and \( \sigma_{\varepsilon}^2 \) and covariance \( \sigma_{\xi \varepsilon} \). We use a time step which resolves the local time scales of the turbulence; viz. \( \Delta t = 0.1 \min(z_{\text{ref}}, L/u_c) \) for (1) and \( \Delta t = 0.1 \min(T_i, L/u_c) \) for (3) and calculate concentration statistics over \( N = 10^6 \) realisations. We treat the source as a steady continuous point source at a height \( z_{\text{ref}} \approx 0.46 \text{ m} \), and calculate the vertical profile of the crosswind integrated mean concentration at a distance \( 100 \text{ m} \) downstream of the source from

\[
C' (z) = \frac{1}{\Delta z N} \sum_{i=1}^{N} \frac{1}{|r_i|}
\]

(8)

where the sum is over the \( n(z) \) particles which cross the plane \( x = 100 \text{ m} \) in a height range \( \Delta z \) centred on the height \( z_i \), and \( u_i \) is the streamwise velocity of the \( i \)-th particle at the time of crossing [9]. Similarly, we calculate the streamwise flux of SO2 from

\[
\bar{w}v' (z) = \frac{1}{\Delta z N} \sum_{i=1}^{N} \frac{u_i}{|r_i|}
\]

and use analogous expressions to calculate the components of the flux due to the mean flow and the turbulence, \( UC' \) and \( w'CC' \).

In the absence of deposition to the surface, a zero flux boundary condition is implemented at the roughness height \( z_0 \) by reflecting all trajectories there. If there is deposition to the surface, a non-zero downward flux \( F_0 = w_0CC' \) at \( z_0 \) prescribed in terms of a deposition velocity \( w_0 \) and is implemented [19] by reflecting particles with probability

\[
R = 1 - \left( \frac{z_i}{\pi/2} \right)^\alpha \frac{w_0}{\sigma_{w_i}} / \left( 1 + \left( \pi/2 \right)^\alpha \frac{w_0}{\sigma_{w_i}} \right).
\]

(9)

**Diffusion vs Langevin Models**

Using the diffusion equation (1) and the Langevin equation (3), we have calculated vertical profiles of concentration for downwind distances from 50 to 800 m and for strongly stable, near-neutral and strongly unstable conditions.

![Figure 1. Comparison of crosswind integrated concentration profiles for the diffusion equation and the 2-D Langevin equation for unstable conditions (L = -5 m)](image)

Figure 1 shows vertical profiles for the crosswind integrated concentration at different distances downstream for unstable conditions (\( L = -5 \text{ m} \)). Concentration is plotted on a log axis, while the height is scaled with a reference height that is roughly equal to \( \frac{z}{z_{\text{ref}}} \) for the 2-D Langevin profiles. Actual values of \( z_{\text{ref}} \) are given in the figure caption.

The diffusion solution is about 25\% low at a height of \( z/z_{\text{ref}} \approx 0.5 \). For near neutral conditions (not shown) the difference is about 10\%, while under stable conditions (not shown) (\( L = 5 \text{ m} \)) the difference is negligible. The under-prediction occurs at all distances and so is not a near-source effect due to the finite

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source height, but rather is a systematic failure of the diffusion approximation as the turbulence becomes increasingly inhomogeneous under increasingly unstable conditions. Well away from the surface, the concentration from the diffusion equation is larger than that from the Langevin equation and the difference increases with height. This also occurs under near-neutral conditions and is consistent with the findings of Mooney and Wilson [10].

**Data Analysis**

**Meteorology**

A full suite of micrometeorological profiles was measured concurrently with each of the tracer releases during PPG. We have estimated the turbulence scales $u_*$ and $L$ and the temperature fluctuation scale $\theta_*$ by fitting the Kansas forms [2] for the wind and temperature profiles to the measured profiles in a self-consistent way. This method works best when the roughness length is known.

Although Pasquill [12] makes an unattributed reference to roughness values ranging between 0.006 and 0.01 m, there seem to be no references to direct estimates of $z_0$ for the PPG data. We have taken 16 near-neutral runs and fitted the wind profiles for these to determine $u_*$, $L$ and $z_0$, finding that $z_0$ indeed ranges roughly between 0.006 and 0.01 m, with a mean value of 0.0074 m. Accordingly, here we have used the value $z_0 = 0.008$ m.

Except for a few cases at the extremes of stability, our values for $u_*$ and $L$ agree well with those of Nieuwstadt reported by van Ulden [16].

**Concentration Profiles**

The PPG concentration data consist of crosswind measurements at a height of 1.5 m at distances of 50, 100, 200, 400 and 800 m downstream and vertical profiles at heights from 0.5 – 17.5 m on six masts located 100 m downstream of the source. Most authors report the crosswind integrated concentration $C' z$ , Separate tabulations of $C' / Q$, where $Q$ is the source strength, by Horst et al. [7] and van Ulden at 1.5 m are in excellent agreement and appear to have been corrected for evaporation losses as reported by Barad [1]. Here we use the more complete tabulations of Horst et al.

We have summed or averaged vertical profiles over all masts registering non-zero concentration and converted them to crosswind integrated concentrations by normalizing to the profile value at a height of 1.5 m and then multiplying by the crosswind integrated concentration at 1.5 m. After discarding Runs 14 and 48s, where satisfactory fits to the meteorological or concentration profiles were not obtained, we have 45 concentration profiles.

The scaled concentration $C'/Q$ is independent of $u_*$ [18] and is a function only of $L$ for fixed geometry (i.e. fixed $z_0$, $z_0$ and $x$). A plot of all the vertical profiles shows a general ordering with $1/L$, but with a lot of scatter because the profiles represent the average at most 6, and usually only 2 or 3, points across the plume. Accordingly, we have averaged scaled profiles within different ranges of $1/L$. Particularly for the near-neutrals runs, this yields well-ordered profiles with associated error estimates.

**Comparison of Theory and Observations**

Figure 2(a) compares predictions of the 2-D Langevin model with PPG data for near-neutral conditions $-0.03 \leq 1/L \leq 0.03$. Clearly the model is not diffusive enough, overestimating the ground level concentration by about 40% and correspondingly underestimating dispersion away from the surface. Figure 2(b) shows that good agreement with the data can be obtained by reducing the Schmidt number $Sc = k_{mass}/\kappa_{mass}$ from 0.74 to 0.52 or equivalently, increasing $k_{mass}$ from 0.47 to 0.67; i.e. by increasing the diffusivity by about 40%. Since the diffusion solution depends only on the product $k_{diff}k_{mass}$, for $k_{diff} = 0.41$ the same solution is obtained with $k_{mass} = 0.57$. This confirms the findings of Wilson et al. [18] and Davis [3], but is contrary to the work of Ley [8] and Ley and Thomson [9] who obtained good agreement with the data using the values $k_{diff} = k_{mass} = 0.41$. 

![Figure 2. Comparison of PPG crosswind integrated concentration profiles with predictions of the 2-D Langevin equation for (a) $K = K_0$ and with no deposition; (b) $K = 1.42K_0$ and with no deposition; (c) $K = K_0$ and with deposition. The data points represent the average of a number of runs and the error bars represent ± one standard error on this average.](image-url)
Figure 2(c) shows the effect of deposition on the concentration profiles using a deposition velocity of \( w_d = 0.05 u_* \) and with \( u_* = 0.43 \text{ m}^2\text{s}^{-1} \). Although there is some basis for a deposition velocity of this magnitude, it is quite uncertain and \( u_* \) itself varies from 0.2 to 0.5 \text{ ms}^{-1} \) over the range of stability shown in Figure 2. Nevertheless, it is clear that including deposition of this magnitude gives almost as good agreement with the data as does increasing the diffusivity.

In order to assess whether the magnitude of the deposition as represented in Figure 2(c) is reasonable, we have also calculated the streamwise flux of SO\(_2\), and its components due to the mean flow and the turbulence, at a downstream distance of 100 m. In the absence of deposition the total downstream flux (i.e. the vertical integral of (9)) is conserved and equals the source flux. The flux due to the fluctuating velocity is negative and ranges from about 3 to 7\% of the total flux. The flux due to the mean velocity, which is what is measured, therefore is slightly greater than the source flux.

![Figure 3. Comparison of PPG data for the downstream SO\(_2\) flux due to wind profile as described above and a stretched exponential function fitted to the concentration profile. The solid black line represents the average of all the data and the dashed black lines represent ± one standard error on this average.](image)

Figure 3 shows the crosswind integrated downstream flux due to the mean flow, normalised by the source flux, as a function of the Obukhov length. The points represent the flux calculated from the PPG concentration and mean wind profiles by integrating the product of the Monin-Obukhov function fitted to the wind profile as described above and a stretched exponential function fitted to the concentration profile. The solid black line represents the mean of all the runs, although there is a slight tendency for lower values under stable conditions. Most points lie within ±15\% of the mean, and the dashed black lines represent ± one standard error on the mean. The blue dashed line is for the calculation with no deposition, and is in remarkable agreement with the data. On the other hand, the red dash-dot line representing the calculation with deposition, is more than ten standard errors lower than the data. Thus it is almost certain that deposition is much less than is implied by a deposition velocity of \( w_d = 0.05 u_* \).

**Conclusions**

Numerical calculations show that the diffusion limit is a good approximation to the Langevin solution for the dispersion from a point source near the ground under stable conditions, but becomes increasingly inaccurate as the stability decreases.

The 2-D Langevin equation gives excellent agreement with data from Project Prairie Grass provided the effective diffusivity for matter is increased by about 40\% compared with that for heat. This finding confirms earlier work by Wilson et al. [18] and others [3, 13]. From (6), the value \( Sc = 0.52 \) corresponds to \( C_o = 3.6 \), which is much lower than estimates from direct numerical simulations [15]. Although similar agreement with concentration profiles can be obtained by invoking the effects of deposition to the surface, we have shown that the resultant streamwise flux is then much lower than is observed.

An increase of 40\% in the effective diffusivity of matter has obvious and important implications for surface exchange processes. However, it is difficult to find a mechanism to explain why matter should be transported more efficiently than heat. These findings clearly need to be tested against other data sets.

**References**


