A COMPOSITE PDF OF SCALAR CONCENTRATION IN TURBULENT FLOWS

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Abstract Experimental plume data and physical arguments are used to make the case for a composite probability density function to describe scalar concentration. High concentration tails of the PDF are shown to be well described by a generalized Pareto distribution.

1. INTRODUCTION

One is interested here in the scalar field $\Gamma(x,t)$, where Γ is the concentration, in mass per unit volume, at a position located by vector x at time t, when a contaminant is introduced into a miscible turbulent host fluid. This is an important topic in many industrial processes and environmental concerns including combustion, toxicity and malodor. Concentration reduction is monitored with the probability density function, PDF, $p(\theta;x,t)$ where,

$$p(\theta;x,t)d\theta = \text{prob}\{\theta \le \Gamma(x,t) < \theta + d\theta\}. \qquad (1)$$

It was shown in Chatwin and Sullivan [1989] that (1) could be written as the composite,

$$p(\theta;x,t) = \pi(x,t)f(\theta;x,t) + (1-\pi(x,t))g(\theta;x,t), \qquad (2)$$

where f and g are the PDFs of source and non-source fluid concentration respectively and $\pi(x,t)$ is the probability that the position located by vector x at time t is in contaminated fluid when the molecular diffusivity κ is zero. As $t \to 0$, and before the effects of molecular diffusivity are significant, f and g approach $\delta(\theta-\theta_0)$ and $\delta(\theta)$ respectively when θ_0 is a uniform initial release concentration and $\delta(*)$ is the Dirac delta function. That is the very general, $\kappa = 0$, PDF described in Chatwin and Sullivan [1990] is recovered. For steady source and flow configurations the equivalent statement is that the distance from the source is very small. At large time (or distance downstream in a steady flow) $\pi \to 0$ and $p \sim g$ and the composite nature of the PDF of (2) appears to be lost. It is the intent in this paper to show, using physical arguments and some grid turbulence plume measurements, that the composite nature of the PDF is retained when the source concentration θ_0 of (2) is replaced with a "local" value.

2. THE SHEET-STRAND TEXTURE

When a blob of contaminant is released in a turbulent flow it is pulled out into ever thinning sheets and strands until the thinning is balanced by the thickening due to molecular diffusion. This occurs at a thickness on the order of the conduction cut-off length $\lambda = (\nu\, \kappa^2/\varepsilon)^{1/4}$ which is 10^{-3} - 10^{-4} m in most flows, where ν is kinematic viscosity and ε is the rate of turbulent energy dissipation per unit mass. Direct experimental observation of the contaminant sheet and strand texture is given in Corriveau and Baines [1993] and Dahm et al [1991] in the near source and far downstream regions of high Schmidt number, liquid contaminant jets respectively. The interpretation of (2) with a sheet-strand, high concentration PDF given by f and a background, low concentration PDF given by g for the near field observation is immediate. These observations suggest a similar decomposition into a high concentration sheet-strand PDF and low concentration background PDF further downstream.

Molecular diffusion is a slow process with respect to transport due to turbulent convective motions. This distinction was used in Chatwin and Sullivan [1990] to derive an expression for the distributed moments of concentration PDFs. That α-β description of moments has received a considerable amount of direct and indirect experimental validation and some salient features of that development relevant to the present discussion follow. The α-β moment description depends only on the ensemble average concentration $\overline{\Gamma}(x,t)$ and the two functions $\alpha(t)$ and $\beta(t)$ for a cloud or $\alpha(x)$ and $\beta(x)$, where x is the distance downstream from a continuous source. The interpretation of a "local" concentration scale given by

$\alpha(t)\overline{\Gamma(\mathbf{0},t)}$ and a factor $\beta(t)$ to account for the effects of molecular diffusivity is consistent with a moving source. That is the relatively high concentrations found in the central regions of a cloud are transported by turbulent convective motions over the cloud observed following a time interval over which the cloud has significantly enlarged but during which time interval there is little molecular diffusion. During this process the relatively high concentrations found in the cloud at the earlier time are drawn into sheets and strands found in the cloud at a later time. The sheet-strand structure is regenerated.

One feature of note in the α-β moment description, that will be used for reference in what follows, is the PDF that corresponds to these moments. Sullivan and Ye [1996] showed that this PDF is,

$$p(\theta;x,t) = p_1\,\delta(\theta-\theta_1) + (1-p_1)\,\delta(\theta-\theta_2), \qquad (3)$$

where,

$$\theta_1(x,t) = \beta(t)\alpha(t)\overline{\Gamma}(\mathbf{0},t) + \theta_2(x,t), \qquad (4)$$

$$\theta_2(x,t) = (1-\beta(t))\overline{\Gamma}(x,t), \qquad (5)$$

and,

$$p_1(x,t) = \frac{\overline{\Gamma}(x,t)}{\alpha(t)\overline{\Gamma}(\mathbf{0},t)}\,. \qquad (6)$$

It was shown in Sawford and Sullivan [1995] that for a non-uniform source (as would correspond to a "moving source") the α-β moment description is recovered but with a slight (10-20%) dependence of α on moment order. A modification to (3) given in Sullivan and Ye [1995] using a convolution shape function led to a biGaussian PDF. This composite PDF was shown to well represent the measured data over the core regions (within 1 ½ half widths and at least until the center-line mean concentration was reduced to half of the release value) of the flows considered. The data was taken from point and line source, grid turbulence, plumes and from a buoyant, cross-flow from a round jet protruding into the logarithmic turbulent boundary layer in a wind tunnel.

3. WIND TUNNEL PLUME MEASUREMENTS

Measurements by Sawford and Tivendale [1992] of the concentration record within a heated wire, grid turbulence, plume were made available for this study. Significantly, these measurements were well resolved (to a sampling interval of about 2λ) and the record lengths were adequate to satisfactorily observe the PDF high concentration tail behaviour.

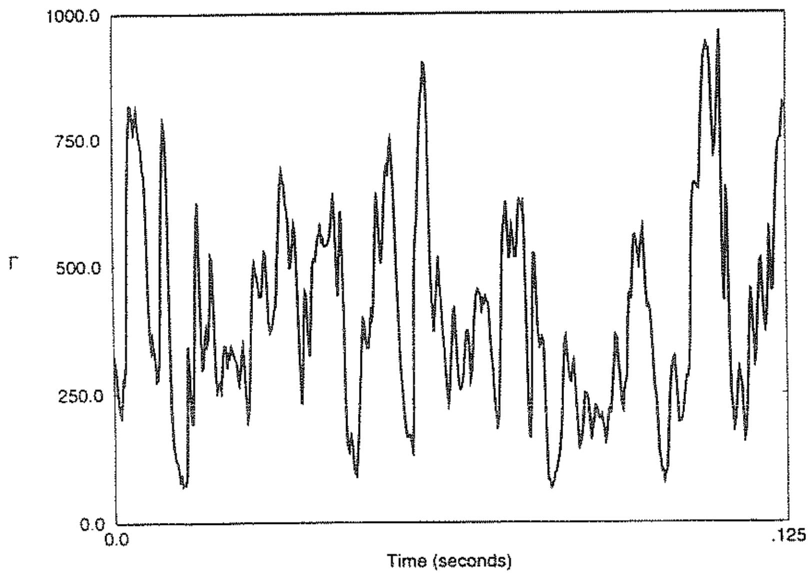

Figure 1

Concentration measurements (in arbitrary units) on the center-line of a plume at 0.7m downstream of a heated wire source in grid turbulence.

The first question to address is whether there is evidence of a sheet-strand texture of order λ width in this order unity Schmidt number ($Sc = \frac{\nu}{\kappa}$) experiment. The typical measured concentration segment, shown on Figure 1, reveals a series of spikes of high concentration. It is worth noting the, isolated, thin, concentration spikes in the Milne and Mason [1991] measurements in the atmospheric boundary layer. The concentration records were decomposed into a record consisting only of high concentration spikes $\Gamma_s(t)$ and the remainder $\Gamma_a(t)$ such that the record,

$$\Gamma(t) = \Gamma_a(t) + \Gamma_s(t)\,; \quad \Gamma_a(t)\Gamma_s(t) = 0\,. \tag{7}$$

There is some subjectivity in selecting the width of spike to be included in $\Gamma_s(t)$ however there was no significant qualitative change apparent to the following results when the spike width was changed. The representative results shown in this paper correspond to a spike width of approximately $U\Delta t \doteq 8\lambda$, where U is the flow velocity. The PDFs of Γ_s and Γ_a are shown in Figure 4. The solid vertical lines shown on Figure 4 are calculated using (3) through (6). The locations and relative probabilities, shown by the heights of the solid lines, are reasonably consistent with the mean and relative proportion of the Γ_s and Γ_a concentrations.

The autocorrelations $R(\tau)$ of the concentration $\Gamma(t)$ can be written as,

$$\begin{aligned} R(\tau) &= \overline{\Gamma(t)\Gamma(t+\tau)} - \overline{\Gamma}^2 \\ &= R_{ss}(\tau) + R_{aa}(\tau) + 2R_{as}(\tau) \end{aligned} \tag{8}$$

using the notation, for example, that,

$$R_{as}(\tau) = \overline{\Gamma_a(t)\Gamma_s(t+\tau)} - \overline{\Gamma}_s\overline{\Gamma}_a \tag{9}$$

It is observed in Figure 2 that substantial correlations do not extend beyond an interval corresponding to the average strand width in $R_{ss}(\tau)$. The correlation $R_{aa}(\tau)$ reflects the procedure of setting $\Gamma_a(t) = 0$ when the $\Gamma_s(t)$ were removed from $\Gamma(t)$ in the decomposition. The $\Gamma_{aa}(\tau)$ is also short-lived and after $\tau > .003$, $R(\tau) \doteq R_{aa}(\tau) + R_{ss}(\tau)$. Without doubt some contribution is unavoidably made to $R_{as}(\tau)$ by the decomposition procedure but there appears to be little correlation between the spikes or between the spikes and the residual, ambient concentration.

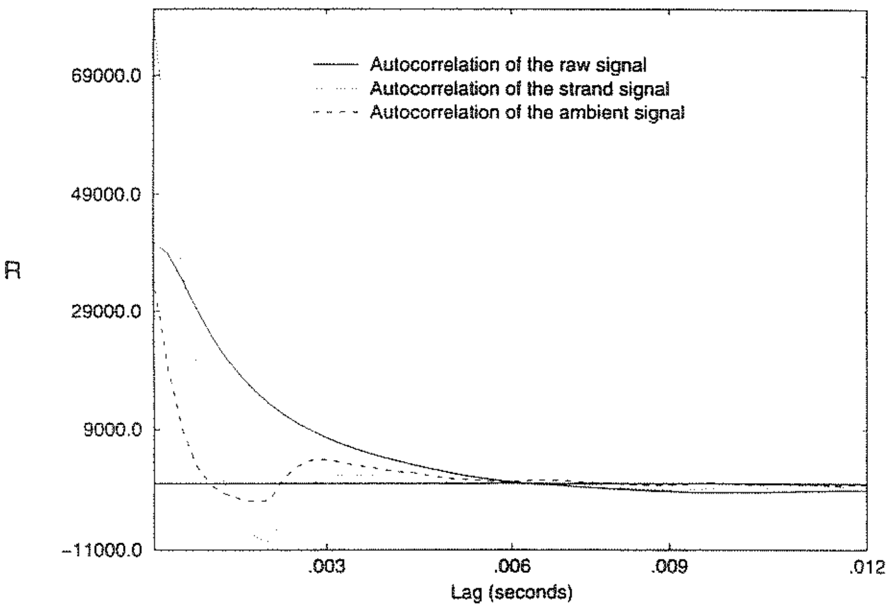

Figure 2
Autocorrelations (in arbitrary units) for the concentration as defined in (8) at the location given in Figure 1.

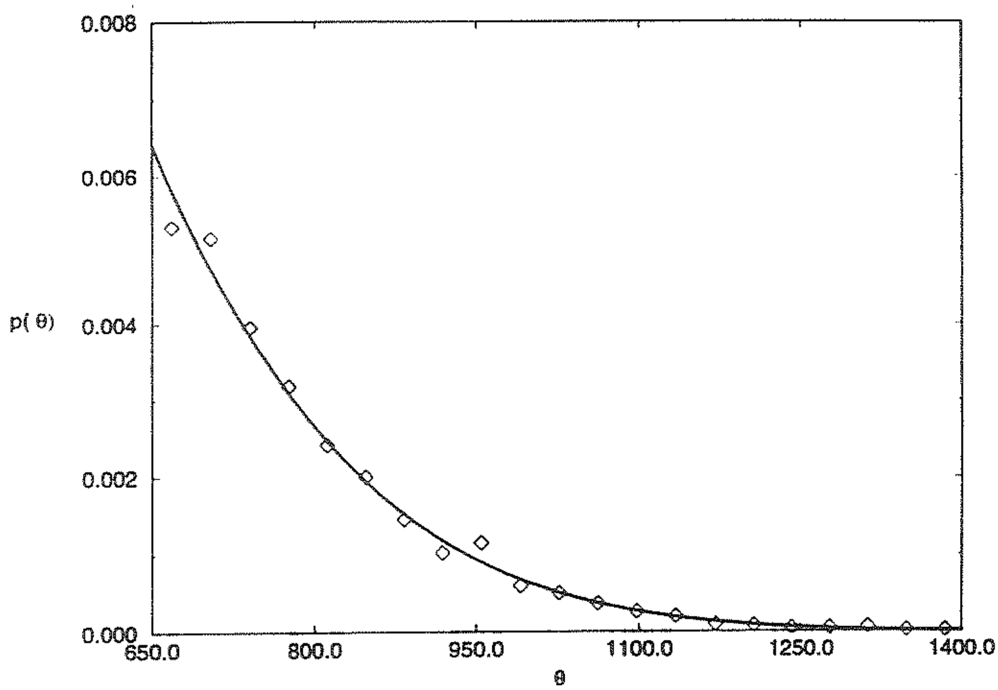

Figure 3
A maximum likelihood estimated fit of the data of Figure 1 (in arbitrary units) with k = 0.142, u = 650 and σ-ku = 155.7.

The high concentration PDF tails that would correspond to the concentration spikes is clearly important. Under rather general conditions, extreme values of independent events tend to a generalized Pareto distribution,

$$G(\theta;\sigma,k) = 1 - \left(1-\frac{k\theta}{\sigma}\right)^{1/k} . \qquad (10)$$

A very good agreement was found in all of the 15 sampling stations for this data. This extremely good agreement, illustrated by the comparison shown on Figure 3, extends from about 25% of the record near the plume center to about 10% near the periphery and the parameter k appears to have the narrow range of values $0.18 \leq k \leq 0.33$. It is of interest to note that Mole et al [1995], using a "declustering" technique and Lewis and Chatwin [1995], without declustering, found very convincing fits of the generalized Pareto distribution for the highest values of concentration data over a wide range of stability conditions in the atmospheric boundary layer. In fact, Lewis and Chatwin [1995] showed a good fit of their data to a composite PDF made up of an exponential and generalized Pareto PDF.

There are many PDFs that will provide a good, high concentration, approximation to the generalized Pareto distribution. One natural PDF, that directly gives the same shape parameter, is the generalized extreme value PDF,

$$f(\theta;\xi,\chi,k) = \exp\left\{\left(1-\frac{k(\theta-\xi)}{\chi}\right)^{1/k}\right\} \qquad (11)$$
$$\frac{1}{\chi}\left(1-\frac{k(\theta-\chi)}{\chi}\right)^{1/k-1} .$$

A comparison of (11) is made with the Γ_s PDF in Figure 4. It is difficult to interpret low concentration measurements due to both the "thresholding" effect where

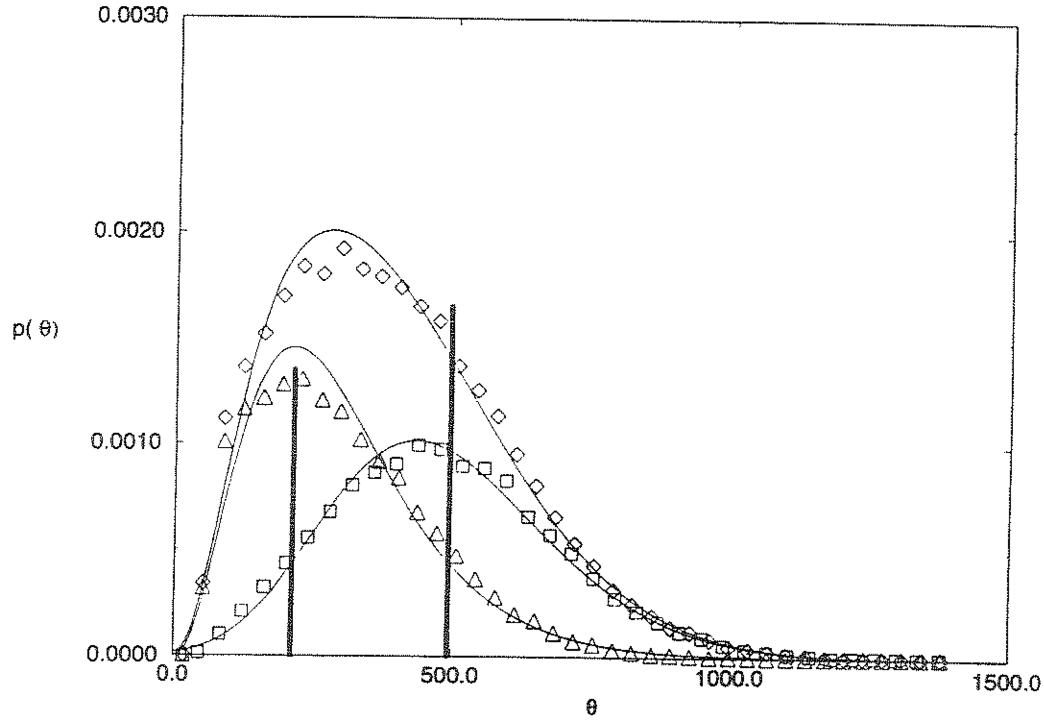

Figure 4
A maximum likelihood estimate of data for Figure 1. The Γ_s data from (7) is fit to (11) ($\xi = 404.575$, $k = 0.150$, $\chi = 181.177$) and the Γ_a data is fit to (12) ($\mu = 3.5085$, $\eta = 84.839$) by calculating the parameters from the first and second moments of $p(\theta;x,t)$ (as would be given by the α-β moment description). The solid bars are the probability from (3) ($\theta_1 = 213.09$, $\theta_2 = 494.37$, $\pi = 0.551$). Concentration θ is in arbitrary units.

instrument noise is comparable with the legitimate signal and the effects of spatial averaging of the transducer. A Gamma density function,

$$g(\theta;\mu,\eta) = \frac{1}{\gamma(\mu)\eta^{\mu}} \theta^{\mu-1} e^{-\theta/\eta} , \qquad (12)$$

where $\gamma(*)$ is the Gamma function, has been selected to fit the low concentration Γ_a and provide the composite distribution shown on Figure 4.

The analysis of this data appears to be consistent with a sheet-strand texture of the concentration record. This naturally leads to a composite PDF made up of a high concentration sheet-strand PDF and a low concentration background PDF. Although a composite made up of a Gamma and generalized extreme value PDF appears to be adequate, other combinations might be usefully explored. One constraint in particular is that $p(\theta;x,t)$ should sensitively depend on only three parameters as discussed in Mole and Clarke [1995]. Ultimately, the parameters can be related to the moments predicted by the α-β description using techniques of Clarke and Mole [1995] and Labropulu and Sullivan [1995] for example. The first and second moments from the α-β description were used to compile (12) and hence the comparison of the composite density function with the data in Figure 4.

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