

# ON MODELLING THE PROBABILITY DENSITY FUNCTION OF CONCENTRATION IN TURBULANT SHEAR FLOWS

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**SUMMARY** The fundamental, and practical, importance of the probability density function of concentration in understanding and analysing turbulent diffusion phenomena is now recognized. One motivation of the work described in this paper was to model theoretically measurements taken in a methane jet. Rather than apply one of a variety of closure hypotheses to the exact evolution equation for the probability density function, a simple and novel approach was adopted in which exact expressions for some basic flows were used as building blocks to construct the probability density function for the jet. Although the method is speculative, the results are sufficiently encouraging for further investigations and applications to be justified.

## 1 INTRODUCTION

Consider a specified ensemble of turbulent flows in which some contaminant (e.g. heat or a foreign fluid) is dispersing. The concentration  $\Gamma(\underline{x}, t)$ , at position  $\underline{x}$  and time  $t$ , of the contaminant, where the units of  $\Gamma$  are arbitrary, is a random variable. This paper deals with  $p(\theta; \underline{x}, t)$ , the probability density function (PDF) of  $\Gamma$ , defined by the following equation which holds for all values of  $\theta_1$  and  $\theta_2$ :

$$P(\theta_1, \theta_2; \underline{x}, t) = \text{prob.}(\theta_1 < \Gamma(\underline{x}, t) < \theta_2) = \int_{\theta_1}^{\theta_2} p(\theta; \underline{x}, t) d\theta. \quad (1)$$

Since  $\Gamma$  is non-negative,  $p(\theta; \underline{x}, t)$  is identically zero for  $\theta < 0$ . The advantages of describing and analysing turbulent diffusion phenomena in terms of  $p(\theta; \underline{x}, t)$  rather than, for example, the ensemble mean concentration  $C(\underline{x}, t)$  or the ensemble mean square fluctuation  $\overline{c^2}(\underline{x}, t)$ , are the explicit recognition that turbulent diffusion is a stochastic process, the fact that the conventional analysis is of little help in many practical problems such as the assessment of flammability risk for a dispersing gas (Chatwin 1982), and the increased information contained in  $p(\theta; \underline{x}, t)$ . Thus  $C(\underline{x}, t)$  and  $\overline{c^2}(\underline{x}, t)$  can be determined from  $p(\theta; \underline{x}, t)$  by the equations

$$C(\underline{x}, t) = \int_0^{\infty} \theta p(\theta; \underline{x}, t) d\theta, \quad (2)$$

$$\overline{c^2}(\underline{x}, t) = \int_0^{\infty} \theta^2 p(\theta; \underline{x}, t) d\theta - C^2(\underline{x}, t), \quad (3)$$

but, conversely, knowledge of  $C$  and  $\overline{c^2}$  is not sufficient to determine  $p$ .

Many measurements of  $p$  have been made in statistically steady flows when  $p \equiv p(\theta; \underline{x})$ . These include the dispersion of heat in turbulent wakes (Larue and Libby 1974) and turbulent jets (Antonia, Prabhu and Stevenson 1975), and the mixing of methane when a natural gas jet is injected into air (Birch, Brown, Dodson and Thomas 1978). Hitherto, theoretical investigations (Dopazo and O'Brien 1976, Janicka, Kolbe and Kollman 1979, Pope 1979) have applied one of a variety of closure hypotheses to the exact evolution equation for  $p$ . The reliability of such methods is uncertain at present, and the present paper summarizes a different method used in an attempt to model the measurements of Birch, Brown, Dodson and Thomas (1978). The method is based on some exact PDFs for some very simple flows, which are then used, as building blocks, to synthesize the PDFs in the flow of interest, using basic physical (but rather speculative) arguments.

## 2 SOME EXACT PDFs

### 2.1 The PDF For A Uniform Strain Field

Townsend (1951) showed, in an investigation of the dispersion of heat spots in isotropic turbulence, that the equation governing  $\Gamma(\underline{x}, t)$  could be solved exactly when the velocity field is a uniform strain with principal rates of strain  $\alpha_1, \alpha_2, \alpha_3$  satisfying (by continuity)  $\alpha_1 + \alpha_2 + \alpha_3 = 0$  and (without loss of generality)  $\alpha_1 \leq \alpha_2 \leq \alpha_3$ . Choosing the directions of the axes  $0x_1, 0x_2, 0x_3$  to be those of the principal rates of strain, Townsend's solution can be written

$$\Gamma(\underline{x}, t) = \frac{2^{3/2} Q}{L_1 L_2 L_3} \exp \left[ -2\pi \left( \frac{x_1^2}{L_1^2} + \frac{x_2^2}{L_2^2} + \frac{x_3^2}{L_3^2} \right) \right], \quad (4)$$

where  $Q$  is the total quantity of contaminant, and

$$L_i^2 = L_0^2 \exp(2\alpha_i t) + \frac{4\pi K}{\alpha_i} [\exp(2\alpha_i t) - 1]. \quad (5)$$

In (5),  $L_0$  is the initial value of  $L_i$ , there is no summation and  $K$  is the molecular diffusivity. Further exact solutions for this flow are given in Saffman (1963). Randomness has to be incorporated for (4) to be relevant in real turbulent flows, but, of course, randomness is naturally present since the axes with respect to which (4) holds have directions which vary from realization to realization of the ensemble. The form of  $p(\theta; \underline{x}, t)$  can be written down as an integral once these directions have been given a probability distribution in space. There is space here only to report the results for two simple cases, but many other examples are treated in detail in Kowe (1982). These cases both arise when the distribution of axes is isotropic in space. For the first,  $L_2 = L_3 > L_0$  in (4), so that the surfaces of constant  $\Gamma$  are flat ellipsoids of revolution (discs), and, for the second,  $L_1 = L_2 < L_0$  in (4), so that the surfaces of constant  $\Gamma$  are thin ellipsoids of revolution (cigars). In these circumstances  $p(\theta; \underline{x}, t)$  is independent of the direction of  $\underline{x}$ , and, for a given value of  $R = |\underline{x}|$ , the maximum and minimum concentrations attainable,  $\theta_{\max}(R, t)$  and  $\theta_{\min}(R, t)$ , are obtained from (4) as

$$\theta_{\min} = A \exp\left(-\frac{2\pi R^2}{L_1^2}\right), \quad \theta_{\max} = A \exp\left(-\frac{2\pi R^2}{L_3^2}\right), \quad (6)$$

where

$$A = A(t) = \frac{2^{3/2} Q}{L_1 L_2 L_3}. \quad (7)$$

Defining  $\omega$  and  $\omega_{\min}$  by

$$\omega = \theta / \theta_{\max}, \quad \omega_{\min} = \theta_{\min} / \theta_{\max}, \quad (8)$$

the forms of  $p$  for the two cases can be written

$$\theta_{\max} p = \begin{cases} (2\theta)^{-1} [\ln \theta_{\min} \ln \theta]^{-1/2}; & \theta_{\min} \leq \theta < 1, \\ 0; & \theta < \theta_{\min}, \theta > 1. \end{cases} \quad (9D) \quad \text{DISCUSSES}$$

$$\theta_{\max} p = \begin{cases} (2\theta)^{-1} [\ln \theta_{\min} \ln (\theta_{\min}/\theta)]^{-1/2}; & \theta_{\min} \leq \theta < 1, \\ 0; & \theta < \theta_{\min}, \theta > 1. \end{cases} \quad (9C) \quad \text{CIGARS}$$

Sketches of  $p$  for these two cases are given in Figure 1. Discussion of the physical reasons for the different shapes are given by Kowe (1982); see also Chatwin and Sullivan (1980).

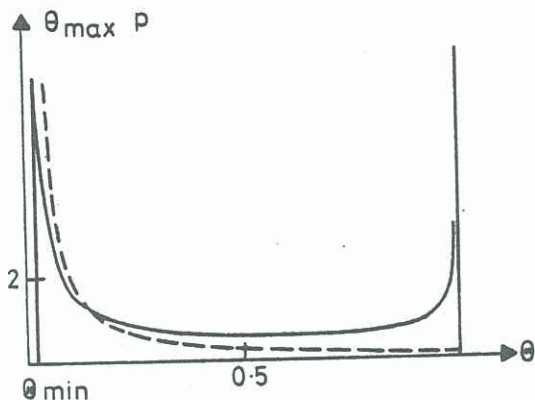


Figure 1 Sketch of the basic  $\theta_{\max} p$  curves in (9D) and (9C) with  $\theta_{\min} = 0.03$ . The solid curve is (9D) and the dashed curve is (9C).

## 2.2 PDFs For Several Dispersing Contaminant Spots

The justification for applying results derived for a uniform strain field to a real turbulent flow is, of course, that this is the relative velocity field in the neighbourhood of any point in a turbulent flow. Many investigations (e.g. Townsend 1951, Batchelor and Townsend 1956, Saffman 1963) have shown that the results derived using this simple field have validity up to a distance of order five times the viscous cut-off length from the point in question. The same field was also used in an investigation of turbulent dispersion by Chatwin and Sullivan (1979). The philosophy behind the modelling procedure summarized in the remainder of this paper is that in the neighbourhood of any point in a turbulent flow, the instantaneous contaminant field in each realization can be represented as the superposition of several spots. The spots have different centres and contain different total quantities of contaminant, but (4) will be assumed to describe the distribution of concentration within each spot, relative to the centre of that spot and with respect to axes along the instantaneous directions of the principal rates of strain at the spot centre.

In applying this philosophy it is necessary to extend the discussion of §2.1 to allow (a) for the random spatial location of the spot centre (meandering), and (b) for the varying total quantities of contaminant within the different spots. Meandering is catered for by giving the distance  $D$  of the spot centre from the fixed coordinate origin a PDF  $f(x)$ , and the varying spot intensity by then giving the quantity  $A$ , defined in equation (7) and appearing in equation (4), a PDF  $g(y)$ . The mathematical procedure and many different cases are discussed in detail by Kowe (1982), but there is space here only to show the typical results in Figure 2. These were obtained with the simple, but natural, choices:

$$\begin{aligned} f(x) &= (2\pi\sigma^2)^{-3/2} \exp(-x^2/2\sigma^2) \quad (0 \leq x < \infty), \\ g(y) &= \beta \exp\{-y - \mu'/2\sigma'^2\} \quad (0 \leq y \leq A_0), \end{aligned} \quad (10)$$

where  $\sigma, \sigma', \mu'$  and  $A_0$  are constants, with  $\beta$  expressible in terms of error functions to ensure that  $g$  is correctly normalized (Kowe 1982). (Note that the form chosen for  $g$  recognizes that  $A$  is essentially positive, and that  $A_0$  is the maximum attainable concentration.) The results of Figure 2 also include some additional simplifications which, however, are introduced only to reduce excessive algebraic and computing complications which seem unlikely to enhance the relevance of the results. Thus, it is assumed throughout that  $L_2 = L_3$ , and, in calculating the effect of the meandering, that the  $x_1$  axis is aligned with the line joining the origin to the spot centre. There is some justification for the first of these simplifications in that calculations by Batchelor and Townsend (1956) suggest that small spots are more likely to be flat than long.

There are several interesting features in the graphs of Figure 2. Here note that for large values of  $R/L_1$  (2g, 2h, 2i), corresponding to PDFs at a relatively large distance from the origin, and also for large values of  $\sigma/L_1$  (2c, 2f, 2i), corresponding to PDFs when the spots are able to wander relatively freely, the PDF is unimodal with a maximum at zero concentration, corresponding to the fact that, in such cases, the most likely encountered concentration is zero. For small values of  $R/L_1$  and high values of  $\mu'/A_0$  (2a, 2b), corresponding to PDFs for relatively small distances from the origin for several spots of high concentration, the PDF is unimodal with the most likely concentration being non-zero. Finally the PDFs in 2d and 2e are bimodal with conditions intermediate between those just described. Further discussion of these graphs is given by Kowe (1982).

## 3 MODELLING PDFs IN A METHANE JET

The qualitative features in Figure 2 that were identified in the preceding discussion are observed in many measurements of PDFs. In particular, bimodal PDFs are observed (e.g. Antonia, Prabhu and Stevenson 1975, Birch, Brown, Dodson and Thomas 1978), the shape of the PDF varies significantly with position  $x$ , and even unimodal PDFs are not usually approximately Normal or log-Normal. PDFs like those shown in Figure 2 were therefore used in an attempt to match the observations of Birch, Brown, Dodson and Thomas (1978). These are shown by the dashed lines in Figure 3, and were taken in a jet of methane injected into ambient air at a distance of 10 jet diameters downstream, and at the various radial positions indicated in Figure 3.

Many methods of modelling these PDFs are possible; that adopted is based on the suggestion in Kent and Bilger (1976) that the PDF in a jet is given by

$$p(\theta; \underline{x}) = [1 - I(\underline{x})] p_n(\theta; \underline{x}) + I(\underline{x}) p_t(\theta; \underline{x}), \quad (11)$$

where  $I(\underline{x})$  is the intermittency (defined to be the probability that the point with position vector  $\underline{x}$  is in the turbulent part of the jet), and  $p_n$  and  $p_t$  are themselves PDFs representing contributions from the non-turbulent and turbulent parts of the jet respectively. Using cylindrical polar coordinates  $(r, \phi, x)$ , it is known that the intermittency is self-preserving and therefore a function only of  $\eta = r/x$ . Based on observations by Corrsin and Kistler (1955) in a heated jet,  $I(\underline{x})$  is taken here to be

$$I(\eta) = \frac{1}{2} [1 - \text{erf}(23.25\eta - 4.39)], \quad \eta = r/x. \quad (12)$$

Many workers using (11) - Kent and Bilger (1976) for example - have taken  $p_n$  to be a delta function. However experimental evidence in e.g. Venkataramani, Tutu and Chevray (1975) has shown that  $p_n$  is broader than a delta function. Here, somewhat arbitrarily,  $p_n$  is taken to be one of the PDFs in the family illustrated in Figure 2, namely that with  $R/L_1 = 0.1, \sigma/L_1 = 0.4\sqrt{2}$ ,  $\mu'/A_0 = 0.25$  and  $\sigma'/A_0 = 0.05\sqrt{2}$ . This distribution has the mean and variance  $0.0226 A_0$  and  $0.002 A_0^2$  respectively. The form chosen for  $p_t$  is one of the same family, namely that with  $R/L_1 = 0.1, \sigma/L_1 = 0.05\sqrt{2}$ , and  $\mu'/A_0$  and  $\sigma'/A_0$  chosen so that  $p(\theta; \underline{x})$  has the measured mean and variance. This

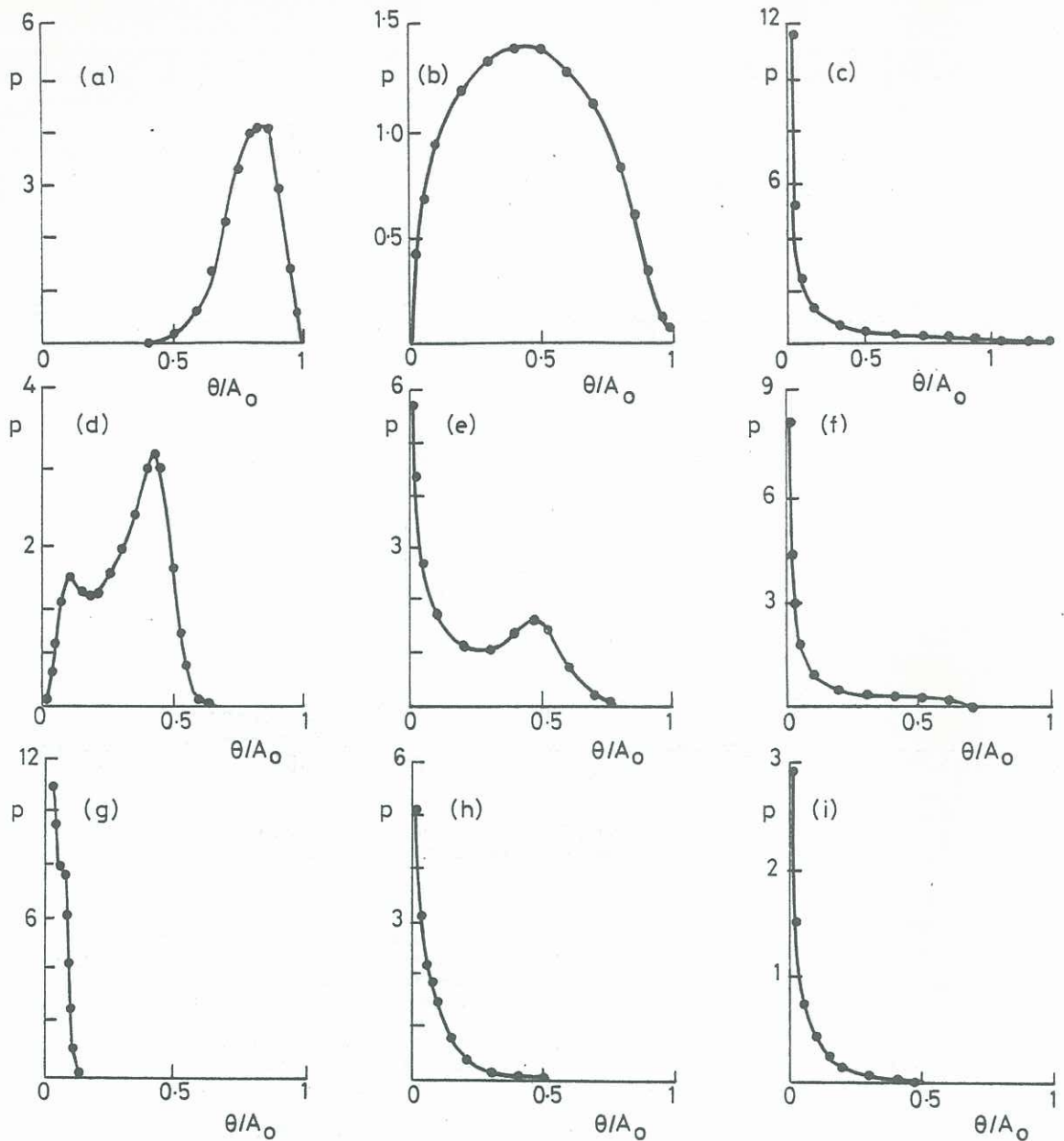


Figure 2 Some illustrative plots of  $p(\theta; \bar{x}, t)$  for several wandering blobs, obtained (as summarized in the text) by extending the basic PDF in (9D) to allow for the effects of meandering and variable maximum concentration using the subsidiary PDFs in (10).

- (a), (b), (c) have  $R/L_1 = 0.1$ ,  $\mu'/A_0 = 0.9$ ,  $\sigma'/A_0 = 0.05\sqrt{2}$  with:  
 (a)  $\sigma/L_1 = 0.05\sqrt{2}$ , (b)  $\sigma/L_1 = 0.15\sqrt{2}$ , (c)  $\sigma/L_1 = 0.4\sqrt{2}$ .  
 (d), (e), (f) have  $R/L_1 = 0.5$ ,  $\mu'/A_0 = 0.68$ ,  $\sigma'/A_0 = 0.05\sqrt{2}$  with:  
 (d)  $\sigma/L_1 = 0.05\sqrt{2}$ , (e)  $\sigma/L_1 = 0.15\sqrt{2}$ , (f)  $\sigma/L_1 = 0.4\sqrt{2}$ .  
 (g), (h), (i) have  $R/L_1 = 0.8$ ,  $\mu'/A_0 = 0.25$ ,  $\sigma'/A_0 = 0.05\sqrt{2}$  with:  
 (g)  $\sigma/L_1 = 0.05\sqrt{2}$  (h)  $\sigma/L_1 = 0.15\sqrt{2}$  (i)  $\sigma/L_1 = 0.4\sqrt{2}$ .

form for  $p_t$  is, of course, like that in Figure 2a. The results of using these choices of  $p_n$  and  $p_t$  are shown by the solid curves in Figure 3. The general agreement is reasonably good, with the model curves reproducing the observed changes in shape as the location moves away from the axis. The major difference between the two sets of curves is that the measured PDFs tend to be smoother; this may be due to the smoothing effect of instrumentation as discussed for example in Chatwin (1982).

#### 4 CONCLUSIONS

Further applications of the PDFs introduced in section 2 are possible, including the modelling of the smoothing effect of instrumentation. Some discussion of these applications is given in Kowe (1982). However, it has

to be recognized that the procedure adopted in section 3 contains too many arbitrary choices to be entirely satisfactory, so that there is need for further work into physically sensible ways of reducing this arbitrariness. Nevertheless, such work seems justified in view of the reasonable agreement between theory and experiment shown, for example, in Figure 3, and because of the absence (at present) of any simple and reliable alternative.

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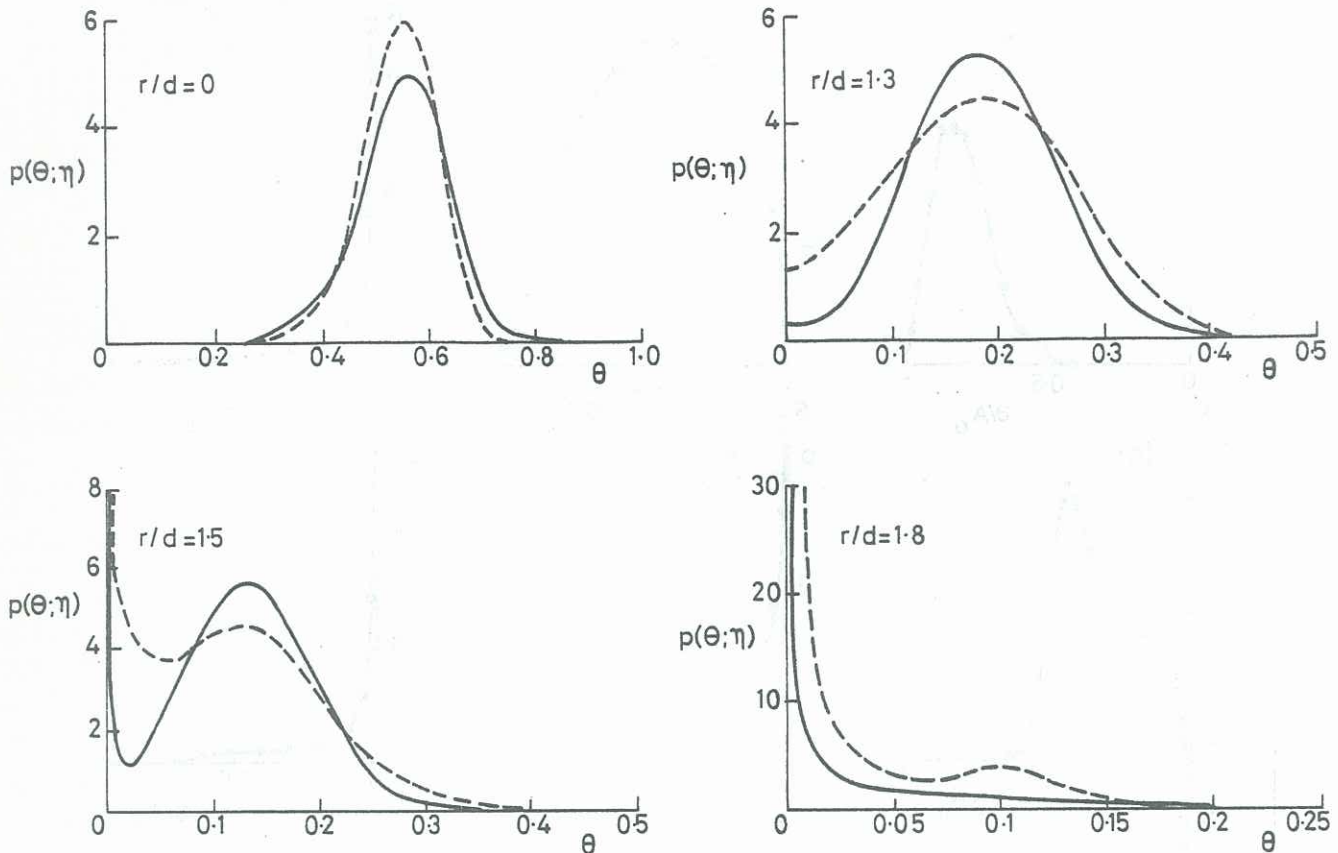


Figure 3 Comparisons between measurements of  $p(\theta; \eta, t)$  in a methane jet (dashed curves) at various radial positions with  $x = 10d$  ( $d$  is jet diameter), and simulations (solid curves) obtained as summarized in the text.

## 6 REFERENCES

ANTONIA, R.A., PRABHU, A. and STEVENSON, S.E. (1975) Conditionally Sampled Measurements in a Heated Turbulent Jet. *J.Fluid Mech.*, 72, 455-480.

BATCHELOR, G.K. and TOWNSEND, A.A. (1956) Turbulent Diffusion. Article in *Surveys in Mechanics* (Editors: G.K. Batchelor and R.M. Davies). Cambridge University Press.

BIRCH, A.D., BROWN, D.R., DODSON, M.G. and THOMAS, J.R. (1978) The Turbulent Concentration Field of a Methane Jet. *J.Fluid Mech.*, 88, 431-449.

CHATWIN, P.C. (1982) The Use of Statistics in Describing and Predicting the Effects of Dispersing Gas Clouds. *J.Haz.Mat.*, 6, 213-230.

CHATWIN, P.C. and SULLIVAN, P.J. (1979) The Relative Diffusion of a Cloud of Passive Contaminant in Incompressible Turbulent Flow. *J.Fluid Mech.*, 91, 337-355.

CHATWIN, P.C. and SULLIVAN, P.J. (1980) The Structure of the Probability Density Function of Concentration in Turbulent Diffusion. *Proc. 13th AIAA Fluid and Plasma Dynamics Conf.*, Snowmass, Colorado.

CORRSIN, S. and KISTLER, A.L. (1955) The Free Stream Boundaries of Turbulent Flows. NACA TN 3133, Washington D.C.

DOPAZO, C. and O'BRIEN, E.E. (1975) Statistical Treatment of Non-isothermal Chemical Reactions in Turbulence. *Combustion Sci. & Tech.*, 13, 99-122.

JANICKA, J., KOLBE W. and KOLLMANN, W. (1979) Closure of the Transport Equation for the Probability Density Function of Turbulent Scalar Fields. *J.Non-equil. Thermodyn.*, 4, 47-66.

KENT, J.H. and BILGER, R.W. (1976) The Prediction of Turbulent Diffusion Flame Fields and Nitric Oxide Formation. *Proc. 16th Int. Symp. on Combustion*, The Combustion Institute, 1643-1656.

KOWE, R. (1982) The Probability Density Function of Concentration in a Turbulent Shear Flow. Ph.D. Thesis, University of Liverpool.

LARUE, J.C. and LIBBY, P.A. (1974) Temperature Fluctuations in the Plane Turbulent Wake. *Phys.Fluids*, 17, 1956-1957.

POPE, S.B. (1979) The Statistical Theory of Turbulent Flames. *Phil.Trans.Roy.Soc.*, A219, 529-568.

SAFFMAN, P.G. (1963) On the Fine-Scale Structure of Vector Fields Convected by Turbulent Fluid. *J.Fluid Mech.*, 16, 545-572.

TOWNSEND, A.A. (1951) The Diffusion of Heat Spots in Isotropic Turbulence. *Proc.Roy.Soc.*, A209, 418-430.

VENKATARAMANI, K.S., TUTU, N.K. and CHEVRAY, R. (1975) Probability Distributions in a Round Heated Jet. *Phys. Fluids*, 18, 1413-1420.