The Interdependence of Some Moments of the PDF of Scalar Concentration

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EXTENDED ABSTRACT

A quantity of miscible contaminant gas is released into the atmospheric boundary layer and the objective is to describe the evolution of contaminant concentration values within the cloud. Although turbulent convective motions will spread the contaminant cloud over distances of tens of meters the only mixing between host and contaminant fluid, and hence reduction of concentration values, takes place through molecular diffusion over length scales of about a millimeter. The normal way to observe the state of concentration values is through the probability density function (PDF) p(2;**x**,t) defined as

$$p(\theta;\mathbf{x},t)d\theta = \text{prob}\left\{\theta \le \Gamma(\mathbf{x},t) < \theta + d\theta\right\}, \quad (1)$$

where ϶(**x**,t) is the concentration, in units of mass per unit volume, at the position located by vector **x** at time t. p(2;**x**,t) is very difficult to theoretically predict or to measure for a cloud even in a well controlled laboratory flow. The approach to be taken here is to invert some relatively few lower-ordered moments, defined as,

$$\mu_n(\mathbf{x},t) = \int_0^\infty (\theta - m_1(\mathbf{x},t))^n\, p(\theta;\mathbf{x},t)d\theta, \quad (2)$$

where,

$$m_n(\mathbf{x},t) = \int_0^\infty \theta^n p(\theta;\mathbf{x},t)d\theta, \quad (3)$$

to approximate the PDF.

A rather simple prescription has been put forward for the distributed moments of (2). For example the second, distributed, central, moment is

$$\mu_2(\mathbf{x},t) = \beta(t)^2 m_1(\mathbf{x},t)(\alpha(t)m_1(\mathbf{0},t) - m_1(\mathbf{x},t)), \quad (4)$$

where ∀(t) and ∃(t) are functions of time that depend on the flow and initial release configuration. This prescription of distributed moments has received considerable validation over a range of steady laboratory flows and release conditions. However there is insufficient experimental information available to directly validate that simple prescription in experiments.

In yet another, related, proposal it was suggested that all of the normalized higher moments $K_n = \mu_n \mu_2^{-n/2}$ could be simply expressed as polynomic functions of the skewness K_3. For example, kurtosis K_4 is

$$K_4 = aK_3^2 + b, \quad (5)$$

where a and b are order one constants. A very important feature of this proposal is that measured values at isolated points throughout the entire concentration field collapse onto a single curve such as that given by (5). There has been experimental validation of (5) over a remarkably wide range of experiments including steady contaminant release from elevated sources in the atmospheric boundary layer covering a variety of stability classes and also in gas clouds of various densities in the laboratory even in the presence of crenellated and un-crenellated fences. The expression given in (5) has also been confirmed with laboratory measurements on a plume in grid-turbulence. Over all of these diverse experimental configurations the constants that appear in (5) are essentially confined to the narrow range of $1 < a < 3$ and $1 < b < 3$.

The aim is to use well controlled laboratory data from a plume in grid turbulence to validate the expressions for K_5 and K_6. It is shown that the parameters that are necessary for the former proposal for the simple prescription for distributed moments can be approximately extracted from the latter proposal for the normalized moments. A framework is provided for the approximate representation of p(2;**x**,t). The validation of the proposed normalized higher moments now implies the validation of the simple distributed moment proposal upon which the PDF is constructed. That is one can use some isolated fixed point data in field measurements to indirectly confirm the appropriateness of this procedure to approximate the PDF.

1. INTRODUCTION

Mole and Clarke (1995) suggested that higher normalized moments, found throughout an entire contaminant concentration field, should collapse onto simple polynomic functions of skewness. The first few of these are:

$$K_4 = aK_3^2 + b$$
$$K_5 = cK_3^3 + dK_3 \qquad (6)$$
$$K_6 = eK_3^4 + fK_3^2 + g$$

where [a,...g] are constants. The remarkable collapse of field data (Lewis et al 1997) and of data from laboratory experiments on dense clouds (Chatwin and Robinson 1997) for kurtosis as a quadratic function of skewness given in (6) is very encouraging. That data was acquired in difficult circumstances both with respect to amount of stationary record and temporal and spatial resolution concerns. The fact that all of the data from isolated fixed point measurements can be used on one graph is very helpful with respect to the inevitable measurement error.

It is essential that the expressions given in (6) be tested with well-controlled and resolved laboratory measurements. Data from experiments on plumes in grid turbulence undertaken by Sawford and Tivendale (1992) will be used to confirm the relationships given in (6).

The motivation for the expressions given in (6) by Mole and Clarke (1995) was the very simple expressions for distributed moments put forward in Chatwin and Sullivan (1990) and modified in Sawford and Sullivan (1995). This simple prescription of distributed moments has received considerable validation in steady laboratory flows. The six lowest order central moments of that prescription are:

$$\mu_2 = \beta^2 C\left(r_2 - C\right)$$
$$\mu_3 = \beta^3 C\left(r_3 - 3r_2 C + 2C^2\right)$$
$$\mu_4 = \beta^4 C\left(r_4 - 4r_3 C + 6r_2 C^2 - 3C^3\right) \qquad (7)$$
$$\mu_5 = \beta^5 C\left(r_5 - 5r_4 C + 10r_3 C^2 - 10r_2 C^3 + 4C^4\right)$$
$$\mu_6 = \beta^6 C\left(r_6 - 6r_5 C + 15r_4 C^2 - 20r_3 C^3 + 15r_2 C^4 - 5C^5\right)$$

where $r_n = \left(\alpha\lambda_n C_0\right)^{n-1}$, $\lambda_2 = 1$, and $C(\mathbf{x},t) = m_1(\mathbf{x},t)$. The $\beta(t)$ and $\lambda_n(t)$ are functions of t only for a contaminant cloud and distance downstream x only for a continuous source such as a plume. C_0 is the maximum value of mean concentration $m_1(\mathbf{0},t)$ for a cloud (or that value on the cross-section of a steady release at distance x downstream). The distributed moments for a cloud are given in (7) in terms of the mean concentration $C(\mathbf{x},t)$, the function, $\beta(t)$, and one function $r_n(t)$ for each moment. A solution procedure for the functions $\alpha(t)$ and $\beta(t)$ for clouds is provided in Labropulu and Sullivan (1995) and that procedure has received some limited experimental validation when extended to generate $\lambda_3(t)$ and hence the third distributed central moment.

In Schopflocher and Sullivan (2005) a relationship was established between the kurtosis given in (6) and the expression for distributed moments given in (7). By extension (Smith 2005) the approximation

$$\lambda_4 = a^{1/3}\lambda_3^{2/3}$$
$$\lambda_5 = c^{1/2}\lambda_3^{3/2} \qquad (8)$$
$$\lambda_6 = e^{1/5}\lambda_3^{8/3},$$

where a, c and e are the constants that appear in (6), can be established. That is, using isolated fixed point measurements to find a, c and e from (6) one can then use the approximation given in (8) to generate the distributed moments μ_n for n > 3 from (7).

The procedure outlined thus far, to generate low-ordered moments which can then be used to approximate the PDF $p(\theta;\mathbf{x},t)$, represents a significant simplification. The main thrust in this paper will be to assess the validity of (6) and (8) using well-controlled and resolved experimental data.

2. EXPERIMENTAL VALIDATION

The experiments of Sawford and Tivendale (1992) were conducted in a suction wind tunnel with mean wind speed U = 5 ms^{-1}. A grid with mesh spacing M = 0.0254 m was used to produce a turbulent flow with Reynolds number R = UM/μ ≅ 8500 where μ is the kinematic viscosity. A heated, 0.213 mm diameter, wire was stretched across the flow at 12.2 M downstream of the grid and produced a line-source of heat. Temperatures were measured with a cold wire anemometer at sampling positions across the plume at locations from 2 mm to 2.6 m downstream of the heated wire source. A full detailed discussion of the experiments is provided in the original paper by Sawford and Tivendale

(1992) and some analysis in Sawford and Sullivan (1995).

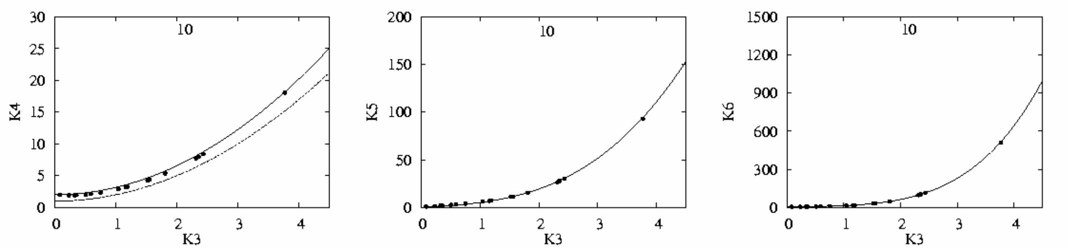
The mean concentration profiles C(x,y) , where x and y are downstream and cross-stream co-ordinates respectively, were observed to be very well approximated by a Gaussian function at each sampling distance downstream. The distributed first four moments were shown to be well described by the expressions given in (7) in Sawford and Sullivan (1995) and also in Sullivan (2004), and the values of α, β, λ_{3E} and λ_{4E} are shown in Table 1. A thorough analysis of the quadratic function relating kurtosis and skewness given in (6) to the moment expressions given in (7) is provided in Schopflocher and Sullivan (2005). Representative fits from the data are shown in Figure 1 (a.....m) and the values of the parameters that appear in (6) from these least square fits are given in Table 2. In the experiments between 2 and 5 repeat measurement sets were made at each downstream sampling station and average values over individual fits are shown in the tables. The variation of parameter values over these replications was small. Distances at less than 10mm downstream of the heated wire were excluded because of resolution problems (see Sullivan 2004) and also data from positions greater than 2σ from the plume center-line, where σ is the cross-stream plume spatial variance, were excluded for reasons of poor signal to noise ratio (see Schopflocher and Sullivan 2002).

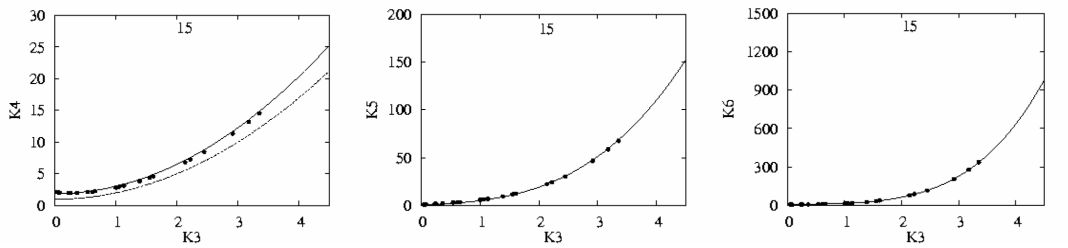
Table 1. Estimates for the λ_n values for the data using (8). The α, β, λ_{3E} and λ_{4E} were obtained from Sawford and Sullivan (1995).

X(mm)	α	β	λ_{3E}	λ_{4E}	λ_4	λ_5	λ_6
10	1.29	0.79	1.04	1.09	1.11	1.18	1.25
15	1.39	0.83	1.05	1.10	1.12	1.20	1.26
20	1.47	0.85	1.06	1.12	1.14	1.21	1.28
30	1.57	0.85	1.07	1.12	1.15	1.23	1.31
50	1.76	0.84	1.07	1.14	1.16	1.24	1.30
70	1.84	0.82	1.08	1.15	1.18	1.27	1.37
100	1.94	0.80	1.08	1.16	1.17	1.26	1.34
150	1.95	0.79	1.08	1.15	1.18	1.28	1.37
200	1.98	0.77	1.08	1.17	1.20	1.32	1.44
300	1.91	0.80	1.09	1.18	1.21	1.33	1.42
700	1.82	0.72	1.08	1.17	1.20	1.39	1.57
1600	1.79	0.62	1.06	1.14	1.22	1.38	1.55
2600	1.56	0.68	1.06	1.13	1.21	1.37	1.50

Table 2. Parameter estimates for the normalized fourth, fifth and sixth moments in (6).

X(mm)	K_4		K_5		K_6		
	a	b	c	d	e	f	g
10	1.14	2.02	1.51	3.68	2.15	5.39	7.13
15	1.16	1.87	1.51	3.51	2.11	5.55	6.93
20	116	1.84	1.51	3.55	2.13	5.51	7.36
30	1.17	1.84	1.55	3.56	2.25	4.87	9.17
50	1.17	1.88	1.54	4.23	2.15	8.56	6.77
70	1.20	1.82	1.66	3.11	2.59	1.52	16.9
100	1.19	1.98	1.59	4.78	2.34	9.02	9.49
150	1.22	1.97	1.71	4.28	2.66	6.31	14.5
200	1.25	2.07	1.85	4.45	3.20	4.33	19.9
300	1.25	2.18	1.84	5.41	2.88	14.0	6.68
700	1.29	1.98	2.37	3.84	5.25	-3.54	26.0
1600	1.44	2.10	2.63	2.76	5.66	-3.66	22.7
2600	1.43	2.22	2.53	4.54	4.94	8.58	11.5


10
K4
K3
K5
K6
(a)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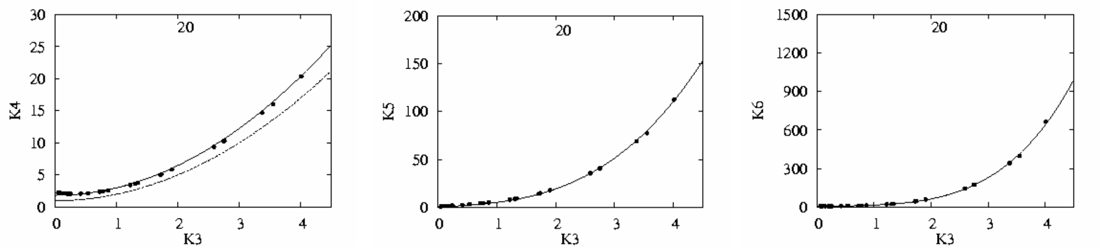
K4
K3
K5
K6
(b)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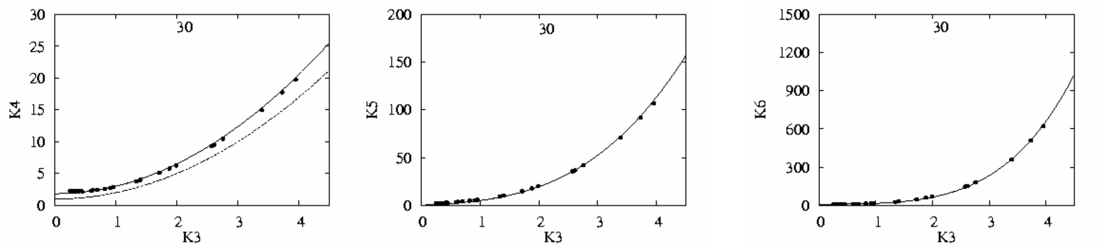
K4
K3
K5
K6
(c)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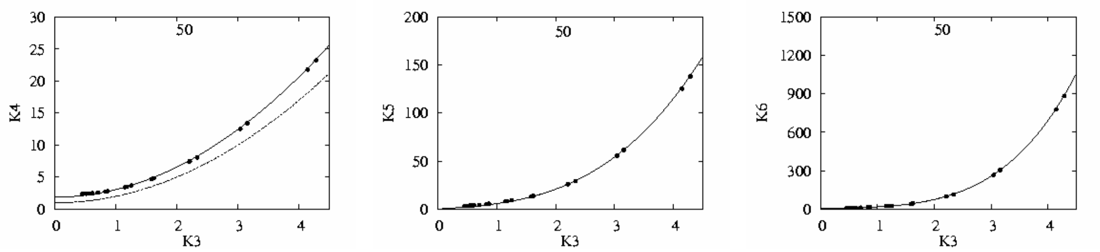
K4
K3
K5
K6
(d)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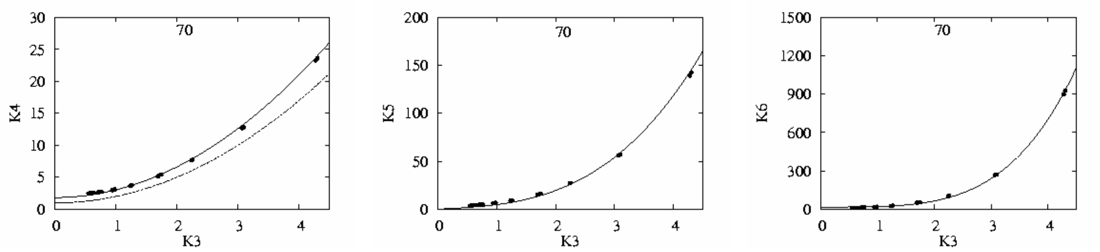
K4
K3
K5
K6
(e)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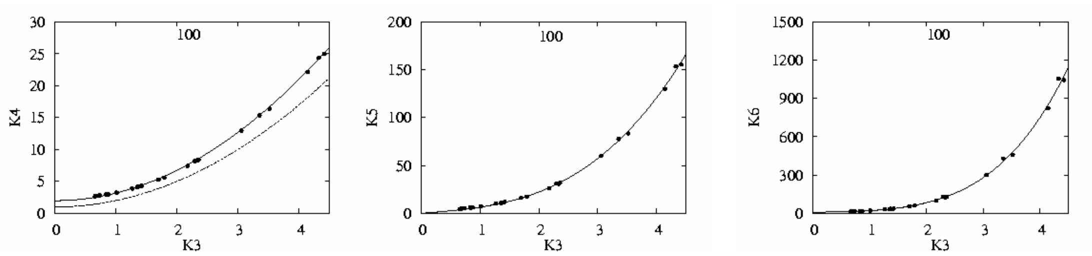
K3
K5
K6
(f)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K3
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K5
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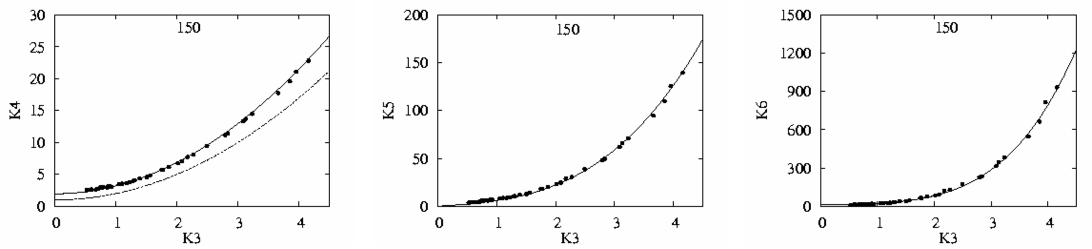
K6
K3

(g)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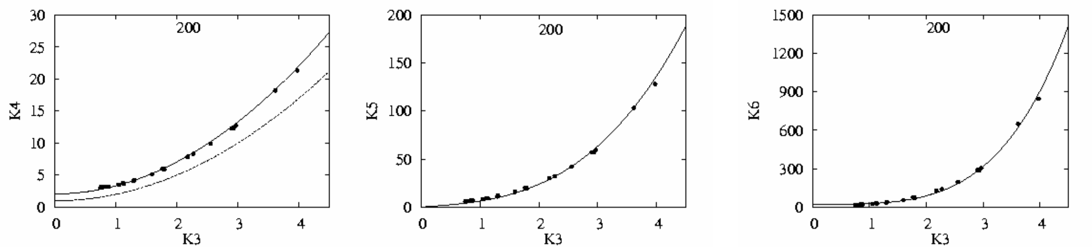
K3
150
K5
K3
150
K6
K3

(h)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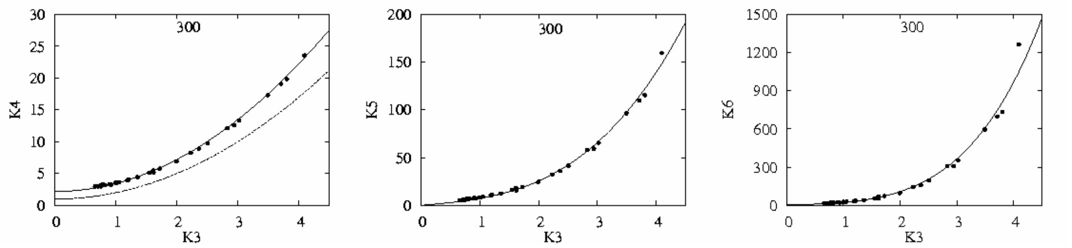
K4
K3
200
K5
K3
200
K6
K3

(i)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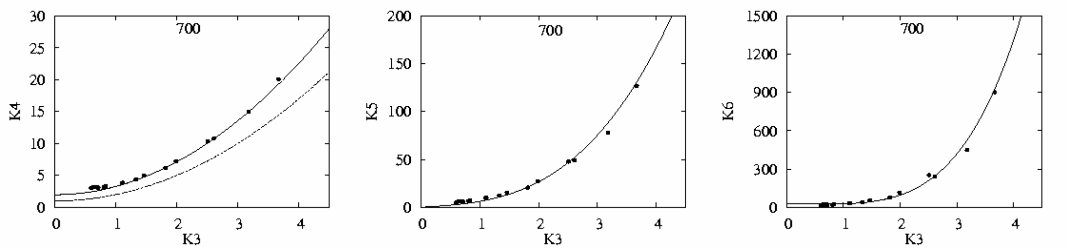
K4
K3
300
K5
K3
300
K6
K3

(j)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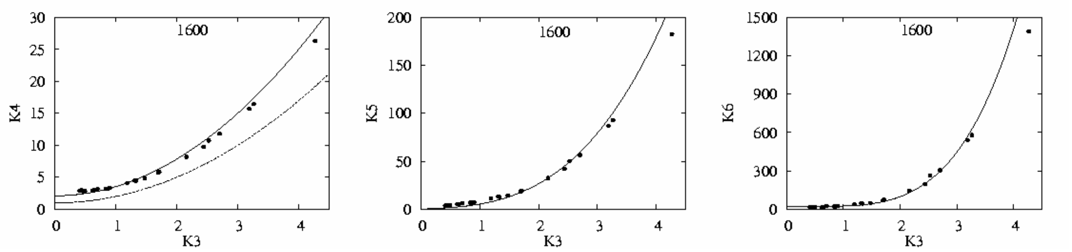
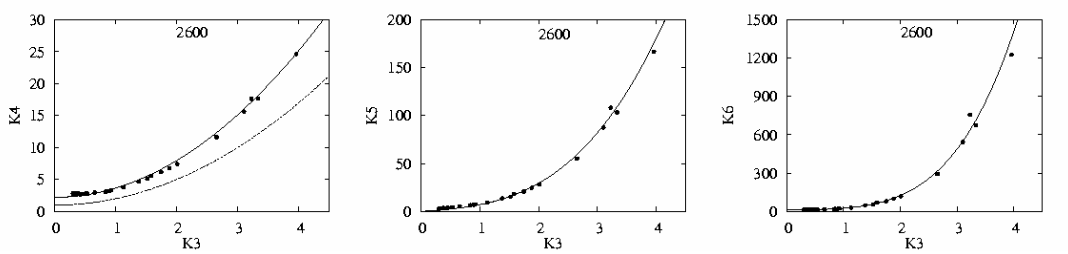
K4
K3
700
K5
K3
700
K6
K3

(k)


1600
K4
K3
1600
K5
K3
1600
K6
K3

(l)



(m)

Figure 1. Graphs showing the least squares fit (solid line) of (6) to the data. The dashed line is the theoretical lower bound $K_4 = K_3^2 + 1$ for all P.D.F.s.

In Figures 1a...m the data are shown to be well represented by least-square curves from (6) for each of the downstream stations. The parameters shown in Table 2 exhibit a slight, systematic, trend as one goes downstream and this trend is consistent with the explanation given in Schopflocher and Sullivan (2005). It is of interest to note the relatively small range of values for the parameters over all of the experimental locations and particularly those that appear in (8). That is $1.14 \leq a \leq 1.44$, $1.51 \leq c \leq 2.63$ and $2.11 \leq e \leq 5.66$. Mole and Clarke (1995) (their Figure 4) found, in a least square fit of all of the data from both stable and convective conditions using a steady release from an elevated source in the atmospheric boundary layer, the values of $c = 2.15$ and $d = -2.38$. In those experiments the largest values of K_5 and K_3 were approximately 10,000 and 20 respectively.

In Table 1 the values of λ_4, λ_5, and λ_6 estimated from (8) and using the average values of the parameters a, c and e shown in Table 2 are presented. It would appear in Table 1 that the λ values vary in a systematic way, however, the overall variation of approximately $1.04 \leq \lambda \leq 1.09$, $1.11 \leq \lambda \leq 1.22$, $1.18 \leq \lambda \leq 1.39$, $1.25 \leq \lambda \leq 1.57$ is reasonably small. A comparison can be made between the averaged measured values of λ_{4E} from Sawford and Sullivan (1995) shown in Table 1 and the values calculated from the approximation given in (8) using λ_{3E} and the estimated value for a. The comparison is quite reasonable and particularly so when account is taken of the variation of measured values shown in Figure 3 of that paper and increasingly so as one proceeds downstream.

3. CONCLUDING REMARKS

The main purpose of this paper was to test the Mole and Clarke (1995) relationships given in (6) with well controlled and well resolved laboratory data. Clearly the curves presented in Figure 1, for each measuring station downstream, support their proposal. Indeed, all of the data shown on Figures 1 a...m could be shown on one graph with small amount of variation of data points about a best-fit curve. The very slight trend in the parameter values as one proceeds downstream could be attributable to the close proximity of the measuring stations to the source and hence not a general feature of most sampling conditions. Thus a remarkable simplification is achieved in that moments higher than the third are determined from the third and second central moments and the constant values that apply to the entire concentration field. Further, these constants can be estimated from isolated, fixed point measurements.

In addition, it would appear that the approximation given by (8), that was derived from connecting the expression for normalized moments in (6) to the Chatwin and Sullivan (1990) expression for distributed moments in (7), provides a reasonable result. That is the comparison of the λ_{4E} values with the λ_4 values in Table 1 is acceptable. This is very important in that the simple expression for distributed moments given in (7) would be extraordinarily difficult to validate directly in steady environmental emissions or even for laboratory measurements on contaminant clouds. The implication is that the validation of (6), using isolated fixed point measurements, is an indirect validation of (7) for distributed moments.

The underlying reason for these seemingly general and simple results given in (6), (7) and (8) is suggested in the fine-scale texture of the contaminant concentration field. When contaminant is released from a finite source, turbulent convective motions stretch out the contaminant into sheets and strands of the conduction cut-off length scale. This texture was exploited in Schopflocher and Sullivan (2005) where the PDF was represented as a mixture density function-the five-parameter, double-Beta density function. The dependence of moments higher than the third on the lower ordered moments led Lewis and Chatwin (1996) to successfully represent atmospheric data with a three-parameter mixture PDF consisting of an exponential and a Generalized Pareto density function. The approach to developing a strategy with which to exploit the moment relationships discussed here to arrive at a probability density function will be left to another paper.

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