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Sensitivity to the Mean in a Model for Concentration Fluctuation Moments

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Abstract Assessment of hazards associated with atmospheric releases of pollutants, whether toxic or flammable, requires the modelling of concentration fluctuations in turbulent flows. In particular, it is desirable to be able to model the probability density function (pdf) of concentration. This can be achieved by modelling moments of concentration, and combining them with some prescription of the pdf in terms of the moments. This paper addresses the question of modelling the concentration moments. The approach is based on the proposal (well supported by experimental evidence) by Chatwin & Sullivan [1990a] that the variance and higher moments of concentration can be expressed as functions of the mean concentration μ, and of 2 parameters α and β, which may be functions of spatial position and time. Sullivan and Moseley used a closure to construct a model for α and β, given a model for μ. To develop the model they considered the idealised case of an unbounded, homogeneous turbulent flow, with a Gaussian spatial distribution for μ. In 2 and 3 spatial dimensions this model gave unphysical results. Clarke & Mole [1995] used a different closure to obtain physically sensible results in 1, 2 and 3 dimensions. The present paper outlines this model and the results obtained with Gausssian μ. It then goes on to assess the sensitivity of the results to the assumption of Gaussian spatial variation of the mean. This is accomplished using polynomial approximations to a Gaussian, and more slowly decaying (exponential and algebraic) functions. For moderate times the differences are not significant, falling within the range of uncertainties associated with other aspects of the model, such as the closure constant. At large times, however, there are large differences, even between the Gaussian and the polynomial approximations. In some cases α tends to a finite constant (≤ 2 in nearly all cases) at large times, while in others it grows without limit. The large time behaviour is only approached very slowly though, so for practical purposes it can probably be assumed that the spatial structure of the mean concentration does not have a critical effect.

1. INTRODUCTION

Atmospheric flows are invariably turbulent, i.e. random. Models of the dispersion of pollutants in the atmosphere must, therefore, be constructed to include the effects of turbulence. In particular, the random character of the velocity field and, hence, of the pollutant concentration field, must be incorporated in the modelling. A major target of research into pollutant dispersion is to formulate models for the probability density function (pdf) $p(\mathbf{x}, t)$ of concentration $\Gamma(\mathbf{x}, t)$, where $\mathbf{x}$ is the spatial position and t is time. One way of achieving this is to model the lowest order moments of Γ, which can then be used to derive $p(\mathbf{x}, t)$, e.g. via maximum entropy methods (Derksen & Sullivan [1990]) or by substitution into a specified parametric form such as the lognormal, beta, gamma, or truncated normal. In this paper we consider only the problem of modelling the moments of Γ. Furthermore, we restrict attention to conserved pollutants of the same density as the ambient air, so that they can be considered as passive scalars.

The equation governing the concentration $\Gamma(\mathbf{x}, t)$ is then

$$\frac{\partial \Gamma}{\partial t} + \Upsilon.\nabla\Gamma = \kappa\nabla^2\Gamma, \qquad (1)$$

where κ is the molecular diffusivity and the (random) velocity $\Upsilon(\mathbf{x}, t)$ satisfies the Navier-Stokes equation. (1) leads (Chatwin & Sullivan [1990b]) to the following equation for the absolute moments $E\{\Gamma^n\}$ for $n \geq 2$:

$$\frac{\partial}{\partial t}\int E\{\Gamma^n\}\,dV = -n(n-1)\kappa\int E\left\{\Gamma^{n-2}(\nabla\Gamma)^2\right\}dV, \qquad (2)$$

where the integrals are taken over all space. (2) holds exactly if $\Gamma = o(|\mathbf{x}|^{-(m-1)/n})$ in unbounded regions, where m is the number of spatial dimensions.

2. THE MODEL FOR CONCENTRATION FLUCTUATION MOMENTS

Chatwin & Sullivan [1990a] considered the problem of dispersing passive scalars released from a steady source of uniform concentration in turbulent flows which are self-similar (so that the concentration moments, when appropriately normalised, depend on downwind distance only through normalising length scales for the crosswind coordinates). They postulated that the mean concentration $\mu = E\{\Gamma\}$, the variance of concentration $\sigma^2 = E\{(\Gamma-\mu)^2\}$ and the higher central moments of concentration $E\{(\Gamma-\mu)^n\}$ satisfied, to a good approximation, the following relationships:

$$\sigma^2 = \beta^2\mu(\alpha\mu_0 - \mu) \tag{3}$$

$$\frac{E\{(\Gamma-\mu)^n\}}{\mu_0^n} = A_n\frac{\beta^n}{\alpha}\left[\frac{\mu}{\mu_0}\left(\alpha-\frac{\mu}{\mu_0}\right)^n + (-1)^n\left(\alpha-\frac{\mu}{\mu_0}\right)\left(\frac{\mu}{\mu_0}\right)^n\right], \tag{4}$$

where α, β and A_n are parameters and μ_0 is a local scale for μ (e.g. the largest value of μ in a cross-section). They presented experimental evidence in support of (3) and (4), and more support has subsequently emerged (Sullivan & Yip [1989], Chatwin et al. [1990], Moseley [1991], Sawford & Sullivan [1995]), including for some non-self-similar flows to which their arguments should also apply. In self-similar regimes α and β are constants, but more generally they would be expected to depend on downwind distance for steady releases, and on time t for instantaneous releases. Chatwin & Sullivan [1990a] argued that $A_n^{1/n}$ is O(1). A first approximation would therefore be to set $A_n = 1$. (Equations (3) and (4) then correspond exactly to a pdf consisting of 2 delta functions, and further modifications are needed to derive a realistic pdf—see Ye [1995], Sullivan & Ye [1995].) All central concentration fluctuation moments $E\{(\Gamma-\mu)^n\}$ could then be modelled by modelling α, β and $\mu(\mathbf{x}, t)$.

Sullivan & Moseley constructed a model for the evolution of α and β, given a model for the mean concentration μ (Moseley [1991]). This was based on (2), together with (3) and (4) with $n = 3$ and the closure assumption

$$(\nabla\Gamma)^2 = A\left(\frac{\Gamma-\mu}{\lambda}\right)^2. \tag{5}$$

Here λ is the conduction cut off (i.e. the smallest length scale present in the concentration field) and A is a constant. They dealt only with the idealised case of dispersion in unbounded, homogeneous turbulent flow (as we shall too for model development purposes), and assumed that μ had a Gaussian profile:

$$\mu(\mathbf{x}, t) = \mu_0(t)e^{-\frac{1}{2}\left(\frac{|\mathbf{x}|}{L}\right)^2}, \tag{6}$$

where L is the cloud width and μ_0 is the mean concentration at the cloud centre. The assumption of a Gaussian profile is usually a good one as long as the source (for steady releases) or the release time (for instantaneous releases) are not approached too closely. Two forms were assumed for L: the inertial subrange result for intermediate times (Batchelor [1952]), applicable to relative diffusion in high Reynolds number environmental flows,

$$\left(\frac{L}{L_0}\right)^2 = 1 + \Sigma_0\tau^3, \tag{7}$$

and the large time result for homogeneous turbulence (Batchelor [1949]) (often approximated in wind tunnel grid turbulence),

$$\left(\frac{L}{L_0}\right)^2 = 1 + \Sigma_1\tau. \tag{8}$$

Here L_0 is the initial cloud width, $\tau = 2A\kappa t/\lambda^2$ is the non-dimensional time,

$$\Sigma_0 = \frac{c}{24A^3}\left(\frac{\lambda}{L_0}\right)^2\left(\frac{\lambda}{\lambda_k}\right)^4,$$
$$\Sigma_1 = \frac{1}{2A}\left(\frac{\lambda}{L_0}\right)^2\left(\frac{\kappa_E}{\kappa}\right),$$

c is a constant, $\lambda_k = (\kappa^3/\epsilon)^{1/4}$ is the Kolmogorov microscale for the concentration field, ϵ is the dissipation rate and κ_E is the growth rate of L^2, i.e. an "eddy diffusivity". For an instantaneous cloud release the equations need to be solved in 3 spatial dimensions, for a continuous point source 2 spatial dimensions are required, and for a continuous line source 1 spatial dimension. In the latter two cases the temporal evolution in the model is converted to a downwind evolution through the relation $X = Ut$, where X is the downwind distance from the source and U is the mean windspeed.

In 1 spatial dimension this model generally predicted a rise in α from its initial value of 1 to a maximum, and a subsequent decrease to a value between 1 and 2. (Note that $\alpha < 2$ implies that the variance has a bimodal spatial structure, whereas for $\alpha \geq 2$ it is unimodal.) However, in 2 and 3 spatial dimensions it gave the unphysical result $\alpha < 1$ (implying negative variance at the cloud centre from (3)), and breakdown of the numerical solutions. Clarke & Mole [1995] showed the latter to be associated with a singularity in the evolution equations for α and β, and overcame both these problems by using the following closure, instead of (5):

$$\frac{\lambda^2}{A}E\left\{\Gamma^{n-2}(\nabla\Gamma)^2\right\} = \frac{1}{2}E\left\{\Gamma^{n-2}(\Gamma-\mu)^2\right\} + \frac{1}{2}E\left\{\Gamma^{n-2}\right\}E\left\{(\Gamma-\mu)^2\right\}.$$

3. RESULTS FOR GAUSSIAN MEAN

Figure 1 shows the evolution of α and β using this new closure, for $\Sigma_1 = 1$ and $\Sigma_1 = 100$. In all cases α increases, reaches a peak (in all cases shown this is for τ less

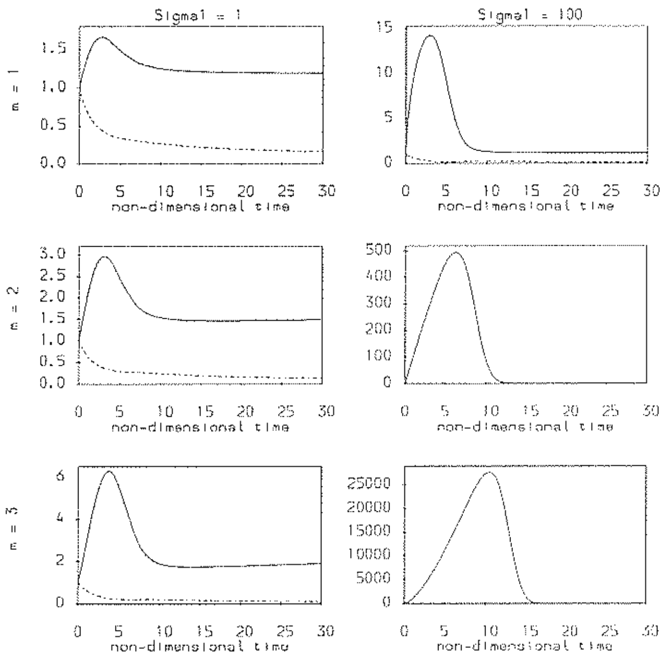

Figure 1: Evolution of α (solid line) and β (dashed line) in non-dimensional time τ. Results are shown for 1, 2 and 3 spatial dimensions, and for $\Sigma_1 = 1, 100$.

than about 10) and then decreases, in all cases reaching a value between 1 and 2 by $\tau = 30$. β generally decreases towards zero, sometimes monotonically, and sometimes with a subsidiary maximum. Larger and later peaks in α result from a higher number of spatial dimensions and from larger Σ values. The results for Σ_0 (not shown) are broadly similar, with larger and later peaks in α than for Σ_1. The largest value of α in Figure 1 is about 27,000 (for $\Sigma_1 = 100, m = 3$). While values of α so far observed are all O(1), it is not clear that large values can be ruled out. In the model the concentration moments remain finite even if $\alpha \to \infty$. Large values of α correspond to a linear rather than quadratic relationship between the variance and the mean (see equation (3)). Chatwin & Sullivan [1990a] suggest that ultimately self-similarity will be attained so α and β become constant, but it is possible that these constants would be very large (α), and very small (β). Furthermore, it has not yet even been tested experimentally whether the $\alpha - \beta$ formulation holds for $m = 3$, so observed α values are not available, and $\Sigma_1 = 100$ is probably unrealistically large. For $\Sigma_1 = 1$ the largest value of α achieved in Figure 1 is about 6, which is certainly consistent with observation.

Integrating for considerably longer times shows that in all cases so far examined α then reaches a minimum at about twice the time at which it achieves its peak. In 1 and 2 dimensions α then appears to tend to constants of approximately 1.18 and 2.0 respectively, while in 3 dimensions α appears to increase without limit. Analysis of the evolution equations confirms these limiting results. We find that, regardless of the assumed growth rate of L, α tends to an asymptotic value, α_∞, as $\tau \to \infty$. If m denotes the number of spatial dimensions, then

$$\alpha_\infty = \begin{cases} \frac{\sqrt{2}}{3\sqrt{3}-4} \approx 1.182 & m = 1 \\ 2 & m = 2 \\ \frac{2\sqrt{2}}{9\sqrt{3}-16} \approx -6.873 & m = 3. \end{cases}$$

A negative value for α_∞ implies that there is no finite limit for positive α, i.e. that α grows unboundedly. These limits imply that cloud centre skewness tends to a negative finite value for a line source, to zero for a point source and to ∞ for an instantaneous release. However, these limits are approached extremely slowly, so they may well have little relevance to problems of practical interest.

4. RESULTS FOR NON-GAUSSIAN MEAN

We have tested the sensitivity of some of these results to the assumption of a Gaussian profile for mean concentration. Let the mean concentration be given by, in centre-of-mass coordinates,

$$\mu(\mathbf{x}, t) = \mu_0(t) g(\phi) \tag{9}$$

where $\phi = |\mathbf{x}|^2/2L^2$. Thus the Gaussian form (6) has $g(\phi) = e^{-\phi}$. We assumed that L was still given by (7) and (8), but chose different forms for $g(\phi)$.

Let $Q_n = \int \mu^n dV$ and $Q = Q_1$. Q is a constant (the amount of pollutant released). If $\dot{}$ denotes $\frac{d}{d\tau}$, then from (9) we have

$$\frac{\dot{Q}_n}{Q_n} = -(n-1)m\frac{\dot{L}}{L}.$$

If we let

$$\hat{Q}_n = \frac{Q_n}{\mu_0^{n-1} Q}$$

then the evolution equations for α and β are:

$$\begin{aligned} \frac{D\dot{\alpha}}{\beta} &= -\frac{m\dot{L}}{L}\Big[2\alpha(1-\beta)(2+2\beta-\beta^2)\hat{Q}_3 \\ &+ \alpha^2\beta^3(\alpha - \hat{Q}_2) + 2(1-\beta)^3\hat{Q}_2\hat{Q}_3 \\ &- 3\alpha(1-\beta)(2+\beta+\beta^2)\hat{Q}_2^2\Big] \end{aligned}$$

$$\frac{D\dot{\beta}}{\beta^2} = \frac{1}{2}\alpha\beta^3(\alpha - \hat{Q}_2) + 3\beta^2(1-\beta)(\hat{Q}_3 - \hat{Q}_2^2)$$
$$- \frac{m\dot{L}}{L}(1-\beta)\left[\alpha\beta(2-\beta)\hat{Q}_2\right.$$
$$\left.+ (1-\beta)\left\{3(1+\beta)\hat{Q}_2^2 - 2(1+2\beta)\hat{Q}_3\right\}\right]$$
$$\frac{D}{\beta^3} = -\alpha\beta(\alpha - \hat{Q}_2) - 6(1-\beta)(\hat{Q}_3 - \hat{Q}_2^2).$$

Thus the evolution of α and β is completely determined by $\dot{L}/L$, $\hat{Q}_2$ and $\hat{Q}_3$. The general form for α_∞ is

$$\alpha_\infty = \frac{\hat{Q}_2\hat{Q}_3}{3\hat{Q}_2^2 - 2\hat{Q}_3},$$

and letting

$$I_n = \int_0^\infty \phi^{\frac{1}{2}m-1} g^n(\phi) d\phi$$

this becomes

$$\alpha_\infty = \frac{I_2 I_3}{3I_2^2 - 2I_1 I_3}.$$

4.1 Polynomial Approximations to the Gaussian

Figure 2 compares the results for α and β with the Gaussian mean, with those using the following polynomial approximations to the Gaussian:

$$g_1(\phi) = 1 - \phi$$
$$g_3(\phi) = 1 - \phi + \frac{1}{2}\phi^2 - \frac{1}{6}\phi^3$$
$$g_5(\phi) = 1 - \phi + \frac{1}{2}\phi^2 - \frac{1}{6}\phi^3 + \frac{1}{24}\phi^4 - \frac{1}{120}\phi^5.$$

Each of these polynomials was truncated at its zero. For the moderate times shown here the differences are not very great. Up to the peak in α the results are indistinguishable. The straight line portions for α at small times for $\Sigma_1 = 100$ correspond to development which very closely approximates that for $\kappa = 0$. In the latter case $\alpha = \theta_0/\mu_0$, where θ_0 is the source concentration, and for $\Sigma_1 \gg 1$ this implies a gradient $\frac{1}{2}m$ and intercept m for the α plots shown, in good agreement with the numerical results. Dependence on the precise form of the mean only appears at about the time α peaks, when molecular diffusion starts to have a significant effect on the development. α is smaller, and β is larger, than with Gaussian mean. For $g_1(\phi)$, $\alpha_\infty = 1$ for $m = 1, 2, 3$; for $g_3(\phi)$, α_∞ takes the values 1.011, 1.007 and 0.986 for $m = 1, 2$ and 3 respectively; and for $g_5(\phi)$, α_∞ takes the values 1.059, 1.130 and 1.183. In all cases these values are less than those for Gaussian $g(\phi)$, and for $m = 3$ they are finite, giving quite different large time behaviour from the Gaussian case. $g_3(\phi)$ in 3 spatial dimensions shows that the closure does not ensure $\alpha \geq 1$ in absolutely all cases—in this case the minimum value of α is 0.96759 at a non-dimensional time of about 137. Again the results for Σ_0 are very similar.

4.2 Spatial Decay of Mean Slower than Gaussian

We also tested how the model would behave if the decay of μ with $\mathbf{x}$ were slower than Gaussian. We examined exponential decay,

$$g(\phi) = h(\phi) = e^{-\sqrt{\phi}},$$

and algebraic decay,

$$g(\phi) = f_N(\phi) = (1+\phi)^{-N}.$$

In the latter case convergence of $\int \mu^n dV$ for $n \leq 3$ requires $N > 3/2$ (and automatically ensures satisfaction of the condition for (2) to hold exactly, provided concentration fluctuations do not behave pathologically as $|\mathbf{x}| \to \infty$).

Figure 3 shows the results for $h(\phi)$, $f_2(\phi)$ and $f_3(\phi)$, up to $\tau = 100$. Again, the differences are very small up to the peak in α, and then develop a little faster than for $g_1(\phi)$, $g_3(\phi)$ and $g_5(\phi)$. Now α is larger, and β smaller, than with Gaussian mean. Very similar results are obtained for Σ_0.

The limiting values of α for $h(\phi)$ are

$$\alpha_\infty = \begin{cases} 2 & m = 1 \\ -4/5 & m = 2 \\ -8/47 \approx -0.170 & m = 3. \end{cases}$$

Thus, in 2 dimensions $\alpha \to \infty$, whereas in the Gaussian case it has a finite limit. For $f_N(\phi)$ we obtain

$$\frac{1}{\alpha_\infty} = 3\left(1 + \frac{1}{6N-3}\right)\left(1 + \frac{1}{6N-5}\right)\cdots\left(1 + \frac{1}{4N-1}\right)$$
$$- 2\left(1 + \frac{1}{4N-3}\right)\left(1 + \frac{1}{4N-5}\right)\cdots\left(1 + \frac{1}{2N-1}\right)$$

for $m = 1$;

$$\alpha_\infty = \frac{(N-1)(2N-1)}{(N-2)^2 - 3}$$

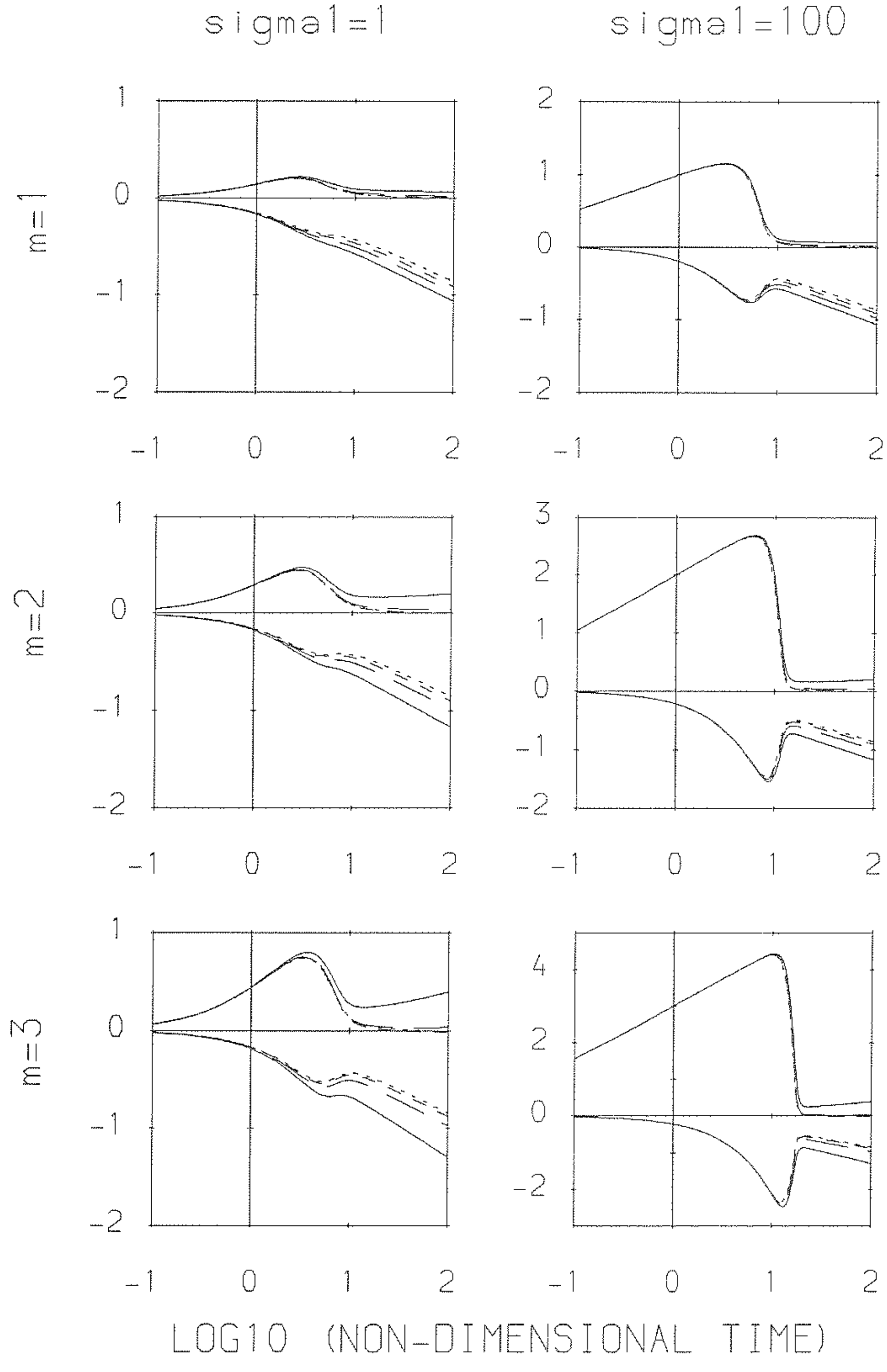

Figure 2: As Figure 1 (except that it is $\log_{10}$ of α, β and τ which are plotted), with Gaussian mean, i.e. $g(\phi) = e^{-\phi}$, (solid line), $g(\phi) = g_1(\phi)$ (short dashes), $g(\phi) = g_3(\phi)$ (medium dashes), $g(\phi) = g_5(\phi)$ (long dashes).

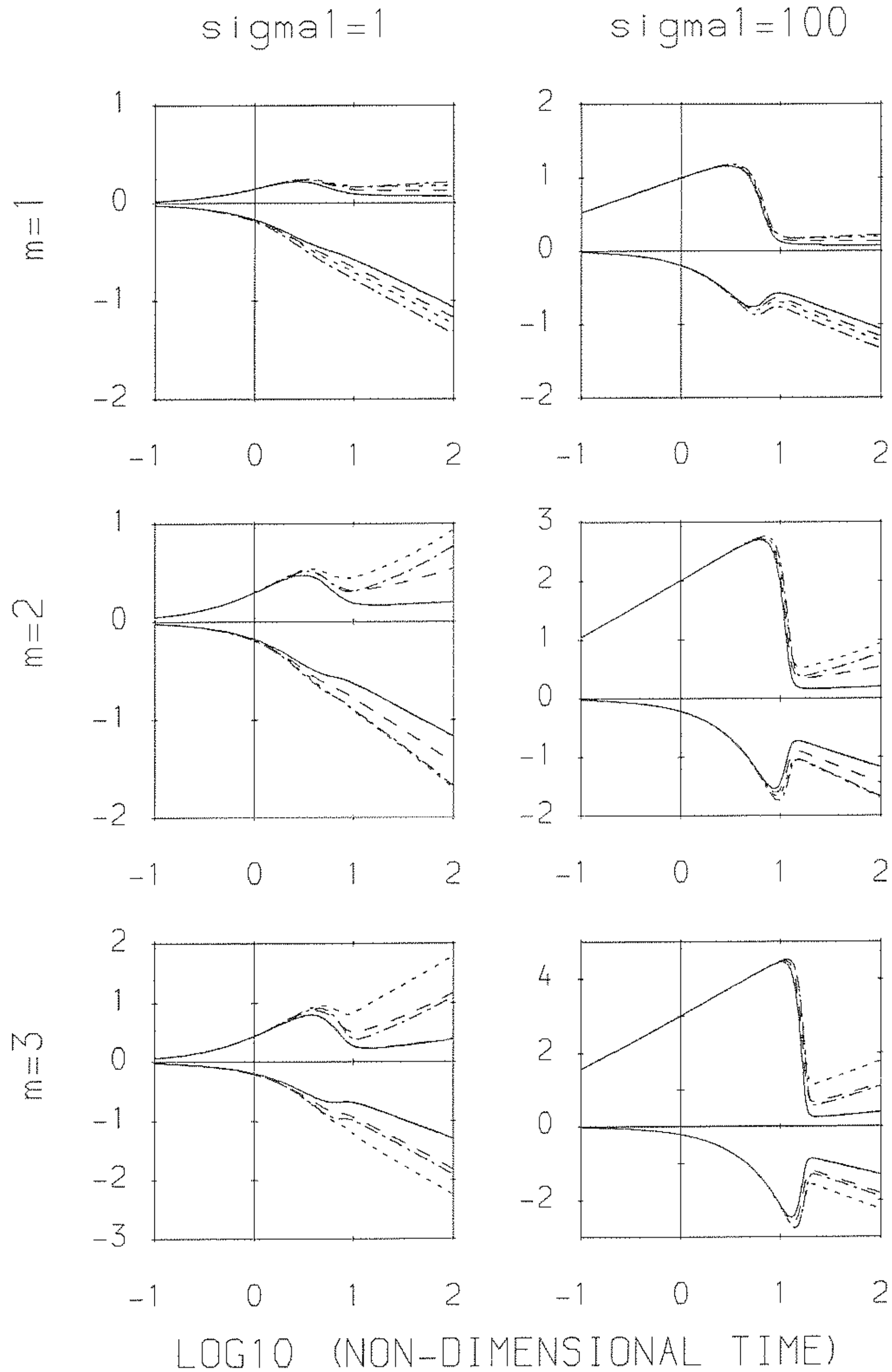

Figure 3: As Figure 1 (except that it is $\log_{10}$ of α, β and τ which are plotted), with Gaussian mean, i.e. $g(\phi) = e^{-\phi}$, (solid line), $g(\phi) = f_2(\phi)$ (short dashes), $g(\phi) = f_3(\phi)$ (medium dashes), $g(\phi) = f_{100}(\phi)$ (long dashes), and $g(\phi) = h(\phi)$ (dot dashes).

for $m = 2$; and

$$\frac{1}{\alpha_\infty} = 3\left(1+\frac{3}{6N-5}\right)\left(1+\frac{3}{6N-7}\right)\dots\left(1+\frac{3}{4N-3}\right) - 2\left(1+\frac{3}{4N-5}\right)\left(1+\frac{3}{4N-7}\right)\dots\left(1+\frac{3}{2N-3}\right)$$

for $m = 3$. Thus, for example, for $N = 2$

$$\alpha_\infty = \begin{cases} 105/64 \approx 1.641 & m=1 \\ -1 & m=2 \\ -7/64 \approx -0.109 & m=3; \end{cases}$$

and for $N = 3$

$$\alpha_\infty = \begin{cases} 15015/10688 \approx 1.405 & m=1 \\ -5 & m=2 \\ -1001/2880 \approx -0.348 & m=3. \end{cases}$$

Again, these give unbounded growth of α in 2 dimensions, in contrast to the Gaussian case. In the limit $N \to \infty$ the Gaussian result for α_∞ (and also for $\hat{Q}_2$ and $\hat{Q}_3$) is recovered exactly, as is to be expected since $(1+\phi)^{-N} \sim e^{-N\phi}$ in this limit. Figure 3 also gives the numerical results for $f_{100}(\phi)$, which up to $\tau = 100$ cannot be separated from the Gaussian results.

5. CONCLUSIONS

With $h(\phi)$, $f_2(\phi)$ and $f_3(\phi)$ in 2 dimensions α grows unboundedly, in contrast to the Gaussian mean for which $\alpha_\infty = 2$. Conversely, α has a finite limit (< 2) for $g_1(\phi)$, $g_3(\phi)$ and $g_5(\phi)$ in 3 dimensions, whereas for the Gaussian $\alpha \to \infty$. Thus, although the behaviour in all cases is very similar around the peak in α at small times, at large times the model behaviour can be quite different from that obtained with Gaussian mean. This is true even for the polynomial approximations to the Gaussian. On the whole the faster μ decays with $\mathbf{x}$, the smaller the values of α, and the larger the values of β.

However, since such large time behaviour in this simple model is probably not practically relevant, it suggests that the important aspects of the evolution of α and β are not very sensitive to the precise form of the mean. At moderate times the differences produced by differences in the mean would probably not be larger than those resulting from uncertainty in the closure parameter $\lambda/\sqrt{A}$.

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