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Asymptotic solutions of the Erdogan–Chatwin equation

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Erdogan & Chatwin (1967) derived a nonlinear diffusion equation

$$\partial_t c = \partial_z([D_0 + (\partial_z c)^2 D_2]\,\partial_z c)$$

which models the effect of buoyancy upon the longitudinal dispersion of a solute in pipe flow. The same equation arises more widely as a limiting form in which only the first buoyancy correction is retained. In this paper long-term asymptotic solutions are obtained both for the smearing-out of a concentration jump and for the approach to normality of a finite discharge. A variant of the method provides an approximate solution to the initial-value problem, and a comparison is made with Prych's (1970) experimental results.

1. Introduction

G. I. Taylor's two papers (1953, 1954) provide the basis for most subsequent fundamental studies of contaminant dispersion in flows. Prior to that work the use of diffusion equations was merely empirical and it was not understood why the effective longitudinal diffusivity could be several orders of magnitude greater than the laminar or turbulent diffusivity κ_3. Formally, the one-dimensional longitudinal dispersion coefficient can be related to the variation across the flow of the concentration c and the longitudinal velocity w:

$$D = \bar{\kappa}_3 - \overline{(w-\bar{w})\,(c-\bar{c})}/\partial_z \bar{c}. \tag{1}$$

In this equation z is the longitudinal distance and overbars are used to denote the cross-sectional average values. Taylor (1953, 1954) recognized that, after transient severe lateral concentration variations had been smoothed out, the remaining variation $c-\bar{c}$ would be determined by a balance between the competing effects of transverse mixing and transverse shear. If the flow is unaffected by the contaminant this balance leads to $c-\bar{c}$ being directly proportional to $\partial_z\bar{c}$ and inversely proportional to the transverse mixing. Thus the dispersion coefficient is independent of $\partial_z\bar{c}$, and the contaminant dispersion is governed by a linear diffusion equation. Also, for parallel flows, the two contributions to D have respectively direct and inverse dependence upon the laminar or turbulent diffusivities, and for weak diffusive mixing D is dominated by the shear dispersion contribution.

For buoyant contaminants the situation is more complicated (Chatwin 1976; Erdogan & Chatwin 1967). The formal definition (1) of the dispersion coefficient remains the same, as does the Taylor mechanism of a dynamic balance between transverse mixing and transverse shear. However, the shear and the mixing are themselves modified by the presence of the buoyant contaminant. First, the longitudinal concentration gradient $\partial_z \bar{c}$ causes a longitudinal pressure gradient, and so a change in $w - \bar{w}$. Second, the cross-sectional concentration variation $c - \bar{c}$ leads to a secondary flow which augments the diffusive mixing and alters the coefficient of proportionality between $c - \bar{c}$ and $\partial_z \bar{c}$. The net result of these complexities is that the dispersion coefficient is a function of the concentration gradient.

It is only in exceptional circumstances that exact analytic solutions can be found to a nonlinear diffusion equation with gradient-dependent diffusivity. (For a buoyancy-driven flow with D proportional to $(\partial_z c)^2$, Imberger (1976) found that there exist similarity solutions. However, this diffusivity is unusual in that it does not reduce to the linear case for small concentration gradients.) Hence understanding of the effect of buoyancy upon contaminant distributions has been limited to qualitative considerations or to numerical solutions for particular cases. Barton (1976*a*) attempted to improve this situation by studying the limiting case of the approach to normality for solutions to the Erdogan–Chatwin equation. The essential simplification which permits analytical progress is that for large times the nonlinearity is weak. Unfortunately Barton's work is in error and underestimates the effect of buoyancy. In the present paper we extend and correct Barton's work.

In axes moving with the bulk velocity $\bar{w}$, the model equation derived by Erdogan & Chatwin (1967) takes the form

$$\partial_t \bar{c} = \partial_z([D_0 + (\partial_z \bar{c})^2 D_2]\, \partial_z \bar{c}), \tag{2}$$

where D_0 and D_2 are constants. The original derivation was as a truncated series expansion in powers of the concentration gradient for a buoyant contaminant in pipe flow. More generally, for that class of flows in which the dispersion coefficient depends upon the magnitude but not the direction of the concentration gradient, (2) is the limiting form when the nonlinearity is weak (e.g. longitudinal dispersion in a straight channel of small depth-to-width ratio; see Smith 1976). The same equation arises without truncation, but with the approximation implicit in the Taylor mechanism, for the transverse dispersion of a buoyant contaminant in open-channel flow (Prych 1970).

The problems addressed in this paper concern the weak buoyancy limit. First of all the general solution procedure is set forth. It is then used to derive approximate solutions for the initial-value problem. In particular, a new calculated value for D_2 (Smith 1979) is shown to yield much improved agreement with Prych's (1970) experimental results. Next formal asymptotic solutions are determined for the approach to normality of a finite discharge and for the eventual smearing-out of a concentration jump. In both these problems it is found that the effect of buoyancy is larger than might be suggested by an order-of-magnitude estimate of the corresponding nonlinear term in the Erdogan–Chatwin equation (2). Heuristically, this unexpectedly large response can be attributed to a resonance between the nonlinear term and a natural decaying mode of the linear equations.

2. Hermite series representation

For a cloud of passive solute, Chatwin (1970) showed that the long-term asymptotic behaviour of the concentration distribution can be described either by a series expansion in powers of $t^{-\frac{1}{2}}$ or by a Hermite series. Barton (1976*a*, *b*) used the former method to study the approach to normality of solutions both to the model equation (2) and to the full hydrodynamic equations for a buoyant contaminant in pipe flow. Here we use the latter method and restrict our attention to the Erdogan–Chatwin equation (2).

Motivated by the form of the eventual Gaussian solution, we pose the Hermite series representation

$$\bar{c} = \frac{M}{\sigma(2\pi)^{\frac{1}{2}}} \sum_{n=0}^{\infty} \frac{a_n(t)}{n!} \mathrm{He}_n(z/\sigma) \exp\{-\tfrac{1}{2}(z/\sigma)^2\}. \tag{3}$$

Here the source strength M is defined to be the integral of $\bar{c}$ with respect to z, so the leading coefficient a_0 equals 1. The defining property of the Hermite polynomials is that

$$\mathrm{He}_n(y) \exp(-\tfrac{1}{2}y^2) = (-d/dy)^n \exp(-\tfrac{1}{2}y^2),$$

i.e. the polynomials are orthogonal with respect to the Gaussian weight function over the infinite interval $(-\infty, \infty)$. If $\sigma(t)$ is chosen to be the exact standard deviation, then $a_2 = 0$ and the expression (3) is the statistical representation of the contaminant distribution in terms of its cumulants, $a_3(t)$ being the skewness and $a_4(t)$ the kurtosis (spikiness).

Our object is to replace all the terms in (2) by Hermite series with the same argument z/σ. It is easy to see that differentiation of the representation (3) with respect to z or t yields similar series. For example,

$$\frac{\partial}{\partial t}\{a_n(t)\, \mathrm{He}_n(z/\sigma) \exp\{-\tfrac{1}{2}(z/\sigma)^2\}\}$$
$$= \left\{\frac{1}{2\sigma^2}\frac{d\sigma^2}{dt} a_n(\mathrm{He}_{n+2} + n\,\mathrm{He}_n) + \frac{da_n}{dt}\mathrm{He}_n\right\} \exp\{-\tfrac{1}{2}(z/\sigma)^2\}.$$

However, the cubic nonlinearity $(\partial_z \bar{c})^3$ presents more difficulty. We need to be able to re-express the sum (including permutations) over i, j and k of the terms

$$-ijk a_{i-1} a_{j-1} a_{k-1} \left(\frac{M}{\sigma^2(2\pi)^{\frac{1}{2}}}\right)^3 \frac{\mathrm{He}_i}{i!}\frac{\mathrm{He}_j}{j!}\frac{\mathrm{He}_k}{k!} \exp\{-\tfrac{3}{2}(z/\sigma)^2\},$$

i.e. a triple product of polynomials in z/σ multiplied by an exponential of three times the desired argument.

Our starting point is Mehler's formula

$$\exp(-\tfrac{3}{2}y^2) = \sum_{m=0}^{\infty} \frac{(-1)^m}{m!\, 3^{m+\frac{1}{2}}} \mathrm{He}_{2m}(y) \exp(-\tfrac{1}{2}y^2) \tag{4}$$

(Erdélyi *et al.* 1953, § 10.13, equation 22). By successively multiplying both sides of this equation by $(\mathrm{He}_i/i!)$, $(\mathrm{He}_j/j!)$ and $(\mathrm{He}_k/k!)$ and at each stage employing the product formula

$$\mathrm{He}_l(y)\, \mathrm{He}_n(y) = \sum_{r=0}^{m} r! \binom{l}{r}\binom{n}{r} \mathrm{He}_{l+n-2r}(y) \quad \text{with} \quad m = \min(l, n)$$

(Erdélyi *et al.* 1953, § 10.13, equation 40), we can represent the triple products.

Thus we have a constructive procedure for determining the constants $G(i,j,k,n)$ in the representation

$$(\partial_z \bar{c})^3 = -\left(\frac{M}{\sigma^2(2\pi)^{\frac{1}{2}}}\right)^3 \sum_{n=0}^{\infty} \left(\sum_{ijk} ijkG a_{i-1} a_{j-1} a_{k-1}\right) \mathrm{He}_n\left(\frac{z}{\sigma}\right) \exp\left\{-\frac{1}{2}\left(\frac{z}{\sigma}\right)^2\right\}. \tag{5}$$

In particular we record that

$$G(2m+1,1,1,1) = (-1)^{m+1}(m-3)/m!\,3^{m+\frac{5}{2}},$$

$$G(2m,4,1,1) = (-1)^{m+1}(m^3-37m+12)/m!\,2^3 3^{m+\frac{9}{2}}.$$

Many of the qualitative properties of G can be seen most readily from the generating function:

$$3^{-\frac{1}{2}}\exp\left(-\tfrac{1}{3}[\xi_1^2+\xi_2^2+\xi_3^2+\xi_4^2-\xi_1\xi_2-\xi_2\xi_3-\xi_3\xi_4-\xi_4\xi_1-\xi_1\xi_3-\xi_2\xi_4]\right) = \sum_{i,j,k,n} \xi_1^i \xi_2^j \xi_3^k \xi_4^n\, G(i,j,k,n).$$

For example, G is invariant under permutations of its arguments and is zero when the sum $i+j+k+n$ is odd.

By this means all the terms in the Erdogan–Chatwin equation are replaced by series of the desired form. Equating coefficients, we obtain the sequence of coupled ordinary differential equations

$$\frac{\sigma^2}{n}\frac{d}{dt}a_n + [a_n + (n-1)\,a_{n-2}]\frac{1}{2}\frac{d}{dt}\sigma^2 = (n-1)\,D_0 a_{n-2} + \frac{D_2 M^2}{2\pi\sigma^4}(n-1)!\sum_{i,j,k} ijk\,G(i,j,k,n-1)\,a_{i-1}a_{j-1}a_{k-1} \tag{6}$$

with $n = 1, 2, \ldots$. It deserves emphasis that these equations are exact and, for the appropriate class of initial conditions, are equivalent to the Erdogan–Chatwin equation.

3. Approximate solutions

For practical purposes it often suffices to know only the simplest global properties of the contaminant distribution, e.g. the standard deviation. Thus solving the full non-linear partial differential equation (2) is not warranted. Indeed, the initial conditions might themselves be known only approximately. The major attribute of the alternative equations (6) is that they readily admit approximate and asymptotic methods of solution. Furthermore, they directly involve the most meaningful statistical quantities, i.e. the standard deviation and the cumulants.

If σ is chosen to be the exact standard deviation (i.e. $a_2 = 0$) then the $n = 2$ equation is of special importance in that it gives the growth rate of the variance σ^2:

$$\frac{1}{2}\frac{d}{dt}\sigma^2 = D_0 + \frac{D_2 M^2}{2\pi\sigma^4}\sum_{i,j,k} ijk\,G(i,j,k,1)\,a_{i-1}a_{j-1}a_{k-1}.$$

The most drastic simplification is to truncate the cubic nonlinearity after the leading term (i.e. to neglect a_j for $j \neq 0$):

$$\frac{1}{2}\frac{d}{dt}\sigma^2 = D_0 + \frac{D_2 M^2}{2\pi\sigma^4}\frac{1}{3^{\frac{3}{2}}}. \tag{7}$$

The implicit solution for $\sigma^2(t)$ is given by

$$\sigma\ \ - A\tan^{-1}(\sigma^2/A) = 2D_0 t + \sigma_I^2 - A\tan^{-1}(\sigma_I^2/A)$$

with

$$A = M(D_2/D_0)^{\frac{1}{2}}\,3^{-\frac{3}{4}}(2\pi)^{-\frac{1}{2}} = 0{\cdot}1750M(D_2/D_0)^{\frac{1}{2}},$$

where σ_I is the initial standard deviation. If for times prior to the validity of the model equation (2) a solution to the complete equations for the flow were available (e.g. Chatwin 1970, appendix C), then it would be appropriate to take σ_I as being the effective, rather than the actual, initial standard deviation.

Prych (1970) gave an order-of-magnitude analysis of (2) which led him to propose an equation of the same form as (7) but with the 30 % larger nonlinear term $D_2 M^2/25\sigma^4$. Using his theoretical estimate for D_2 he found that the theory underestimated the excess dispersion due to buoyancy by about a factor of three. Here the suggested reduction in the nonlinear coefficient would make the disagreement slightly more severe. However, Smith (1979) points out that Prych's quasi-laminar model for the detailed dynamics of the flow is not appropriate. The revised theoretical estimate for D_2 is larger by a factor of $\frac{70}{19}$ and yields a much improved fit with Prych's experiments (see figure 1 below).

There are many alternative ways of trying to improve upon the approximation (7), none of which seem to lead to exact analytic solutions. One of the simpler approaches is to regard the nonlinearity parameter $N = D_2 M^2/2\pi D_0 \sigma^4$ as small. To the first approximation the a_{n-2} terms on the two sides of (6) cancel each other out. Thus we find that the cumulants $a_n(t)$ are related to their (effective) initial values by the linear solution $a_n^I(\sigma_I/\sigma)^n$. Using this simple result, and making the further assumption that the cumulants are moderately small, we can estimate the nonlinear term in the equation for the variance

$$\frac{1}{2D_0}\frac{d\sigma^2}{dt} = 1 + \frac{N}{3^{\frac{3}{2}}}\left\{1 + \sum_{m=2}^{\infty} (-1)^{m+1}\frac{(2m+1)(m-3)}{m!\,3^m} a_{2m}^I \left(\frac{\sigma_I^2}{\sigma^2}\right)^m\right\}. \tag{8}$$

The neglected terms are of second order either in the nonlinearity parameter or in the cumulants. If it should happen that the precise profile is known rather than just the first few cumulants, then the series can be summed to give

$$\Sigma = -\frac{1}{2M}\int_{-\infty}^{\infty} \bar{c}(0,z)\left[6 + \exp\left(-\frac{1}{2}\left(\frac{z}{s}\right)^2\right)\left\{\left(1+\frac{\sigma_I^2}{s^2}\right)^{\frac{5}{2}} \mathrm{He}_4\left(\frac{z}{s}\right) + 9\left(1+\frac{\sigma_I^2}{s^2}\right)^{\frac{3}{2}} \mathrm{He}_2\left(\frac{z}{s}\right)\right\}\right] dz$$

with $s^2 = \frac{3}{2}\sigma^2 - \sigma_I^2$. The conversion to an integral follows from the definition

$$a_{2m}^I = \frac{1}{M}\int_{-\infty}^{\infty} \bar{c}(0,z)\,\mathrm{He}_{2m}(z/\sigma_I)\,dz$$

and the resulting integrand is summed by means of the formulae

$$(1+\mu^2)^{\frac{3}{2}}\,\mathrm{He}_2(\mu y)\exp(-\tfrac{1}{2}\mu^2 y^2) = \sum_{m=0}^{\infty}\frac{(-1)^{m+1}(2m+1)}{m!}\left(\frac{\frac{1}{2}\mu^2}{1+\mu^2}\right)^m \mathrm{He}_{2m}(y),$$

$$(1+\mu^2)^{\frac{5}{2}}\,\mathrm{He}_4(\mu y)\exp(-\tfrac{1}{2}\mu^2 y^2) = \sum_{m=0}^{\infty}\frac{(-1)^{m}(2m+3)(2m+1)}{m!}\left(\frac{\frac{1}{2}\mu^2}{1+\mu^2}\right)^m \mathrm{He}_{2m}(y).$$

Mehler's formula as quoted in the previous section corresponds to $\mu^2 = 2$.

In Prych's experiment the buoyant contaminant was introduced uniformly over a finite width $b = 2\times 3^{\frac{1}{2}}\sigma_I$. Performing the integration and writing r for the ratio σ_I^2/σ^2, we find that (8) becomes

$$\frac{1}{2D_0}\frac{d\sigma^2}{dt} = 1 + \frac{N}{3^{\frac{3}{2}}}\left\{\frac{3(1-\frac{4}{3}r+\frac{2}{3}r^2)}{(1-\frac{2}{3}r)^{\frac{7}{2}}}\exp\left(\frac{-r}{1-\frac{2}{3}r}\right) - 2\right\}. \tag{9}$$

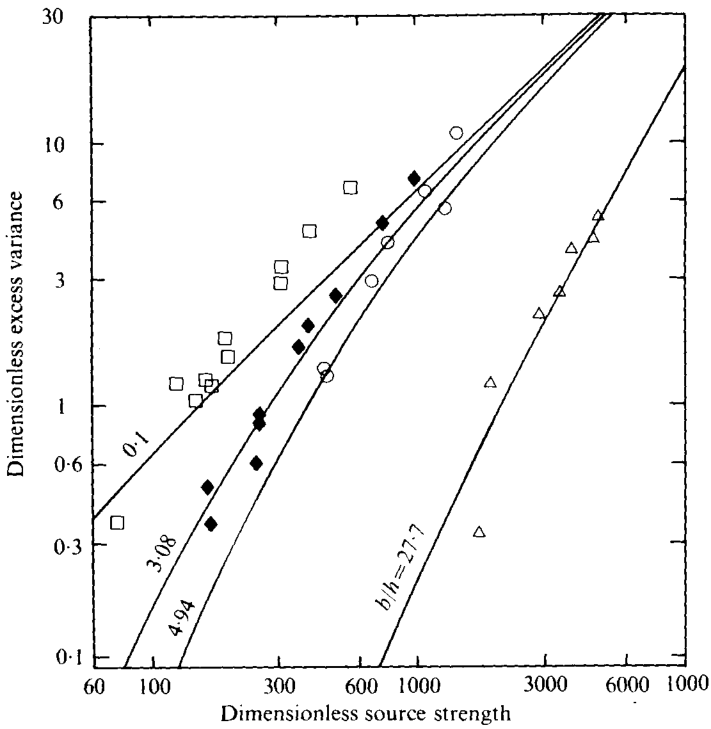

FIGURE 1. Comparison between Smith's (1979) theory and Prych's (1970) experimental results for the excess variance due to buoyancy as a function of the strength and width of the source.

Initially the dispersion is less than that predicted by (7). However, once the contaminant distribution has doubled its width the subsequent evolution is as given by (7). An intuitive explanation of this behaviour is that the extensive region of weak concentration gradients delays the full effect of the nonlinear dispersion. Since the nonlinearity is weak, the identification of the effective initial conditions with the actual initial conditions requires that the Taylor balance is achieved before there is significant distortion of the contaminant distribution (Chatwin 1970). In this context a sufficient condition is that the discharge width exceeds the water depth (Smith 1979).

Equation (9) is a first-order ordinary differential equation and numerical solutions have been obtained using a Runge–Kutta procedure. Figure 1 compares these results with Prych's experimental results as presented in his figures 5.2 and 6.2. If we take $\bar{c}$ to be the fractional density perturbation, then the definition of the dimensionless source strength is Mgh^2/D_0^2, where h is the channel depth. The dimensionless excess variance is the difference, at large distances downstream, between the values of σ^2/h^2 for buoyant and neutrally buoyant contaminants, i.e.

$$\lim_{t\to\infty}(\sigma^2-\sigma_I^2-2D_0t)/h^2.$$

The four groups of experimental results and the corresponding theoretical curves are labelled by the breadth-to-depth ratio of the source.

The main reason for the improvement upon Prych's theory is the use of the revised estimate for D_2 (Smith 1979):

$$D_2 = h^5 g^2/96 u_*^3 k^3.$$

Here u_* is the friction velocity, k the von Kármán constant for the flow and it has again been assumed that $\bar{c}$ is measured in density units. Prych's experiments involved five different flow conditions, and hence five values of the two important turbulence constants k and $\alpha = D_0/hu_*$. In dimensionless form the nonlinearity parameter in (9) is proportional to $(\alpha/k)^3$. Thus it is the average of this quantity that is used in the numerical calculations.

The agreement between theory and experiment deteriorates as the source becomes narrower and as the discharge becomes more buoyant. It happens that these are the conditions under which the approximate equation (8) becomes unreliable (i.e. the nonlinearity parameter is initially large). However, there are also more substantial reasons than just the results of figure 1 for restricting the situations in which (2) is used. Smith (1979) derives a hierarchy of model equations which can be expected to apply in those regimes where the Erdogan–Chatwin equation ceases to be appropriate.

4. Approach to normality

After a sufficiently long time the contaminant distribution evolves according to the linear diffusion equation. Thus one way of regarding the earlier buoyancy-modified evolution is as providing starting conditions for the final linear stage. This is exemplified by Prych's (1970) choice of the excess variance as a practical measure of the buoyancy effects. Since the cloud of contaminants is continually widening, we can infer that the largest-scale effects due to buoyancy occur immediately prior to the linear stage. This is precisely the circumstance in which the Erdogan–Chatwin equation becomes applicable. Hence an analysis of the asymptotic solutions of (2), or equivalently of (6), is pertinent even to problems where the initial concentration gradients are much too large for the uniform applicability of the model equation.

As a preliminary to solving (6) it is convenient to use the equation for σ^2 (i.e. $n = 2$) in order to replace t by σ^2 as the independent variable. Thus, for $n = 1, 3, 4, \ldots$, we have

$$\begin{aligned}\frac{2\sigma^2}{n}\frac{da_n}{d\sigma^2}+a_n &= N(n-1)!\sum_{i,j,k} ijk\,G(i,j,k,n-1)\,a_{i-1}a_{j-1}a_{k-1}\\ &\quad -N\sum_{i,j,k} ijk\,G(i,j,k,1)\,a_{i-1}a_{j-1}a_{k-1}\left[\frac{2\sigma^2}{n}\frac{da_n}{d\sigma^2}+a_n-(n-1)\,a_{n-2}\right],\end{aligned} \quad (10)$$

where we have again used the abbreviated notation

$$N = D_2 M^2/2\pi D_0 \sigma^4.$$

To solve (10) we make the assumption that σ^2 is large (i.e. consider the eventual approach to normality). Thus equations (10) become linear equations with small forcing terms. The homogeneous equations have solutions (integrating factors) which decay as σ^{-n}. An order-of-magnitude estimate of the solutions might suggest that a_n decays at the same rate as the larger of σ^{-n} and the nonlinear forcing. The detailed results obtained below reveal that the dominant effect of buoyancy occurs in a term which does not conform to this general rule.

For the first few cumulants the nonlinear terms are only a small perturbation about the linear solution, and we obtain

$$a_1 = \alpha_3 \left(\frac{D_2 M^2}{2\pi D_0}\right) \frac{1}{4 \times 3^{\frac{5}{2}}} \sigma^{-7} + O(\sigma^{-9}),$$

$$a_3 = \alpha_3 \sigma^{-3} + \alpha_3 \left(\frac{D_2 M^2}{2\pi D_0}\right) \frac{1}{2 \times 3^{\frac{5}{2}}} \sigma^{-7} + O(\sigma^{-9}).$$

Without loss of generality the constant α_1 which one would expect as a multiplier of the free linear solution in the expression for a_1 has been set equal to zero. To do this it suffices to shift the z axis such that at large σ^2 the centroid of the concentration profile is situated at the origin. The similar multiplier α_3 in the expression for the skewness is an undetermined constant which depends both upon the initial skewness of the contaminant distribution and upon the effect at small values of σ^2 of any nonlinear corrections to the Erdogan–Chatwin equation.

In the equation for the kurtosis (i.e. $n = 4$) the dominant nonlinear term has precisely the same σ dependence as the natural decaying mode:

$$\frac{\sigma^2}{2} \frac{da_4}{d\sigma^2} + a_4 = \left(\frac{D_2 M^2}{2\pi D_0}\right) 6G(1,1,1,3)\, \sigma^{-4} + O(\sigma^{-8} \ln(\sigma/\sigma_0)).$$

This resonance leads to a relatively large response

$$a_4 = -\left(\frac{D_2 M^2}{2\pi D_0}\right) \frac{16}{3^{\frac{5}{2}}} \sigma^{-4} \ln(\sigma/\sigma_0) + \alpha_4 \sigma^{-4} + O(\sigma^{-8} \ln(\sigma/\sigma_0)).$$

The role of σ_0 is simply to make dimensionless the argument of the logarithm. For definiteness we define

$$\sigma_0^4 = |D_2|\, M^2/2\pi D_0, \quad \text{i.e.} \quad \sigma/\sigma_0 = |N|^{-\frac{1}{4}}.$$

The form of the error estimate is in fact consequent upon the occurrence of higher-order terms involving a_4 in the equation for a_4. The effect at large values of σ^2 of $(\partial_z \bar{c})^4 D_4$ and further corrections to the nonlinear dispersion can be regarded as being subsumed in this same error estimate.

For the subsequent even cumulants the nonlinearity dominates the free linear decaying solution and we obtain

$$a_{2m} = N \frac{(-1)^m m(m-4)(2m-1)!}{(m-2)(m-1)!\, 3^{m+\frac{1}{2}}} + \alpha_{2m} \sigma^{-2m} + O(\sigma^{-8} \ln^2(\sigma/\sigma_0)).$$

As above, the α_{2m} terms show the extent to which the cumulants are dependent upon the detailed behaviour at small values of σ^2. The size of the error estimate is related to a subsidiary resonance of a higher-order term in the a_8 equation.

Since $\alpha_1 = 0$, the nonlinearity is relatively weak for the odd cumulants. (We recall that G is non-zero when the sum of its arguments is even, and in particular that $G(1,1,1,2m) = 0$.) At $n = 5$ the response is essentially linear:

$$a_5 = \alpha_5 \sigma^{-5} + \alpha_3 \left(\frac{D_2 M^2}{2\pi D_0}\right) \frac{5!}{2^4 3^{\frac{5}{2}}} \sigma^{-7} + O(\sigma^{-9}).$$

At $n = 7$ there is a further resonance:

$$a_7 = -\alpha_3 \left(\frac{D_2 M^2}{2\pi D_0}\right) \frac{7!}{2 \times 3^{\frac{9}{2}}} \sigma^{-7} \ln(\sigma/\sigma_0) + \alpha_7 \sigma^{-7} + O(\sigma^{-9}).$$

For the subsequent odd cumulants the leading term reverts to the σ^{-7} dependence which is suggested by an order-of-magnitude estimate of the nonlinear terms in (10):

$$a_{2m+1} = \alpha_3 \left(\frac{D_2 M^2}{2\pi D_0}\right) \frac{(-1)^{m+1}(m^3 - 37m + 12)(2m+1)!}{2^4 (m-3)\, m!\, 3^{m+\frac{5}{2}}} \sigma^{-7} + O(\sigma^{-9} \ln(\sigma/\sigma_0)).$$

Bringing together all the above asymptotic solutions, we find that the concentration is given by

$$\begin{aligned} \bar{c} = \frac{M}{\sigma(2\pi)^{\frac{1}{2}}} \exp\left\{-\frac{1}{2}\left(\frac{z}{\sigma}\right)^2\right\} \Bigg\{ 1 &+ \sum_{j=3}^{7} \frac{\alpha_j}{j!} \sigma^{-j}\, \mathrm{He}_j \\ &+ N\left[\frac{1}{2 \times 3^{\frac{7}{2}}} \ln|N|\, \mathrm{He}_4 + \sum_{m=3}^{\infty} \frac{(-1)^m (m-4)}{2(m-2)\, m!\, 3^{m+\frac{3}{2}}} \mathrm{He}_{2m}\right] \\ &+ \alpha_3 \sigma^{-3} N \left[\frac{\ln|N|}{8 \times 3^{\frac{9}{2}}} \mathrm{He}_7 + \sum_{m \neq 3} \frac{(-1)^{m+1}(m^3 - 37m + 12)}{2^4 (m-3)\, m!\, 3^{m+\frac{5}{2}}} \mathrm{He}_{2m+1}\right] + O(N^2 \ln|N|) \Bigg\}, \end{aligned} \tag{11}$$

where the Hermite functions have the common argument z/σ. In particular, we note that if there is symmetry with respect to z then for large σ^2 the departure from normality is dominated by the $N \ln|N|$ term. Furthermore, at the next order down (i.e. N or σ^{-4}) the only influence of the initial conditions is via the kurtosis factor α_4.

Figure 2 shows the scaled profiles of $\bar{c}$ for positive values of D_2 with $\alpha_j = 0$. We observe that, as the cloud of contaminant widens, the nonlinearity acts in such a way as to reduce the overall steepness. This is in addition to the augmented rate of spreading. The opposite is the case when D_2 is negative and the buoyancy tends to reduce the dispersion.

If we envisage the asymptotic solutions being used beyond a given variance σ_I^2, then the constants α_j can be related to the cumulants at this inner reference position. To the order of accuracy of the above asymptotic approximations the resulting equation for the standard deviation is

$$\begin{aligned} \frac{1}{2D_0}\frac{d\sigma^2}{dt} = 1 + \frac{N}{3^{\frac{3}{2}}}&\left\{1 + \sum_{m=2} \frac{(-1)^{m+1}(2m+1)(m-3)}{m!\, 3^m} a_{2m}^I \left(\frac{\sigma_I^2}{\sigma^2}\right)^m\right\} \\ &+ \frac{N(a_3^I)^2}{2 \times 3^{\frac{5}{2}}}\left(\frac{\sigma_I^2}{\sigma^2}\right)^3 - N^2 \frac{20}{3^6} \ln(\sigma^2/\sigma_I^2) \\ &- \frac{N^2}{54} \sum_{m=5}^{\infty} \frac{(m-3)(m-4)(2m+1)!}{(m-2)(m!)^2\, 3^{2m}} \left[1 - \left(\frac{\sigma_I^2}{\sigma^2}\right)^{m-2}\right]. \end{aligned} \tag{12}$$

This can be regarded as being an extension of the approximate equation (8), provided that the nonlinearity parameter and the initial cumulants are small enough for the asymptotic formulae to be uniformly applicable. We note that the skewness tends to increase the dispersion, but that the other new terms marginally reduce the variance from the predictions of (8). The oscillatory character of the constants $G(i, j, k, n)$ makes

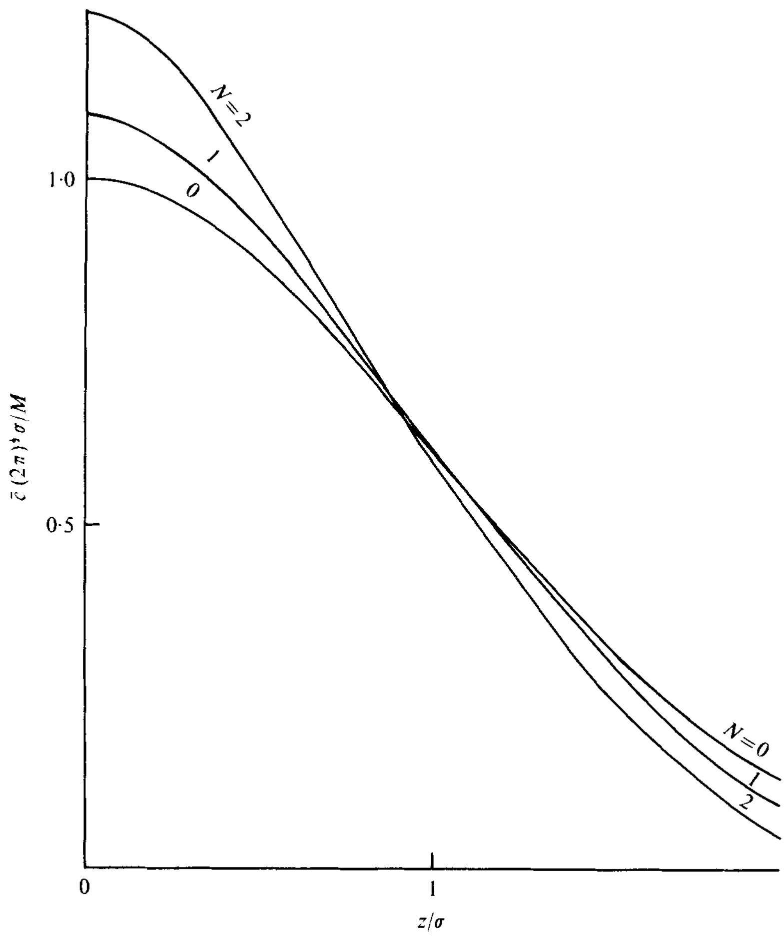

FIGURE 2. Approach to normality of the concentration distribution $\bar{c}$ for symmetric solutions of the Erdogan–Chatwin equation as the nonlinearity parameter N tends to zero (i.e. the standard deviation σ tends to infinity).

it possible to infer that the dominant neglected terms are positive, so (12) slightly underestimates σ^2.

The solution of (12) permits us to revert to the use of t as the independent variable. In particular, we note that after a sufficiently long time σ^2 evolves according to the linear diffusion equation

$$\sigma^2 = 2D_0(t-t_0)+O(t^{-1}).$$

Here t_0 is a virtual time origin, and is an alternative way of representing the excess variance due to buoyancy. This simple formula enables us to confirm that the occurrence of logarithmic terms in the concentration distribution (11) is not merely an artifact of the choice of independent variable.

5. Switchback

Barton (1976*a*, *b*) studied the long-term effect of buoyancy upon dispersion by means of a series expansion of the form

$$\bar{c}(X,T) \sim T^{-1}C^{(1)}(X)+\ldots+T^{-n}C^{(n)}(X)+\ldots$$

with $$X = z/(2D_0 t)^{\frac{1}{2}}, \quad T = (2D_0 t)^{\frac{1}{2}}/\sigma_0.$$

Here the asymptotic co-ordinates (X,T) can be thought of as being first approximations to (z/σ) and to the inverse nonlinearity measure $|N|^{-\frac{1}{4}}$. Barton's results differ from (11) in the absence of the logarithmic terms. This is a serious disagreement because, according to the present analysis, the leading-order effect of buoyancy occurs in the $N\ln|N|$ term. The purpose of this section is to show how Barton's method can be modified to yield correct results, and to explain why certain qualitative conclusions of Barton's papers remain valid.

As has several times been noted above, the logarithmic terms arise as the result of a resonance of a natural decaying mode of the linear equations. Barton overlooked this resonance by assuming that there existed a bounded solution $h(X)$ to the differential equation

$$h_{XX}+Xh_X+5h = -\beta_0^3 Q_2(\alpha R/P\sigma)^2\,\partial_X[X^3\exp(-\tfrac{3}{2}X^2)] \tag{13}$$

[Barton 1976*a*, equation (3.10)], where the expression on the right-hand side arises from the leading-order buoyancy terms. The homogeneous equation has the Hermite-function solution $\mathrm{He}_4(X)\exp(-\frac{1}{2}X^2)$. Thus we can use Sturm–Liouville theory to assert that a necessary condition for $h(X)$ to be bounded is that the integral

$$\frac{1}{4!(2\pi)^{\frac{1}{2}}}\int_{-\infty}^{\infty}\mathrm{He}_4(X)\frac{d}{dX}[X^3\exp(-\tfrac{3}{2}X^2)]\,dX$$

be zero. The actual value of the integral is $2\times 3^{-\frac{7}{2}}$ (i.e. the nonlinear terms resonate with the Hermite function). Hence Barton's calculations are in error and there does not exist a bounded solution for $h(X)$. (Integrating both sides of (13) four times with respect to X gives an equation which can be solved explicitly. The resulting explicit solution for $h(X)$ grows as X^3 for large X.)

The function $\tilde{h}(z/\sigma)$, which describes the next-to-highest-order effects of buoyancy in the representation (11) (i.e. the sum of the N terms), satisfies the equation

$$\tilde{h}_{XX}+X\tilde{h}_X+5\tilde{h} = \partial_X[X^3\exp(-\tfrac{3}{2}X^2)]-2\times 3^{-\frac{7}{2}}\,\mathrm{He}_4(X)\exp(-\tfrac{1}{2}X^2).$$

Apart from a constant factor, this equation differs from (13) in that the resonant part of the forcing has cancelled out. This cancelling can be attributed to the occurrence of the logarithmic term involving $\mathrm{He}_4(z/\sigma)$ earlier in the asymptotic series. In the literature on asymptotic expansions this method of including additional earlier terms to remedy later singularities is called 'switchback' (Chang 1961).

Thus the modification to Barton's method consists of checking rigorously at the T^{-j} stage of the calculation whether a bounded solution $C^{(j)}(X)$ does exist. If not, then an additional earlier term $T^{-j}\ln T C^{(j,1)}(X)$ is needed. The extra terms are multiples of linear eigenmodes, the amplitudes of which are chosen to cancel out the resonance in the $C^{(j)}$ equation. At a higher stage of the calculation powers of logarithms can arise in the same way (e.g. the error estimate in the expression for a_{2m}).

The counterpart to (11) is

$$\bar{c} = \frac{M}{\sigma_0(2\pi)^{\frac{1}{2}}}\exp\left(-\tfrac{1}{2}X^2\right)\Big\{T^{-1}+\beta_3 T^{-4}(X^3-3X)$$
$$\mp 2^{-1}\times 3^{-\frac{1}{2}}T^{-5}\ln T(X^4-6X^2+3) \pm 2^{-1}\times 3^{-\frac{1}{2}}T^{-5}\sum_{m=3}^{\infty}\frac{(-1)^m(m-4)}{(m-2)\,m!\,3^m}\mathrm{He}_{2m}(X)$$
$$+\sum_{j=0}^{6}\beta_j T^{-1-j}\mathrm{He}_j(X)+O(T^{-8}\ln T)\Big\},$$

where the nonlinear buoyancy terms have the upper sign when D_2 is positive. The undetermined constants β_j depend upon the initial contaminant distribution and upon the effect at small values of T of any corrections to the Erdogan–Chatwin equation. One consequence of the nonlinearity is that equation (6.13) of Chatwin (1970) does not hold, and there is no acceleration of convergence if the Hermite series is rearranged into Edgeworth's form.

Although Barton (1976*a*) did not solve (13), he made use of it in a calculation to determine the systematic long-term contribution of the buoyancy terms to the second moment of the contaminant distribution. On the basis of this calculation he reached the important conclusion that the dispersion induced by buoyancy effects at short and intermediate times is of greater order than the dispersion which is induced at asymptotically large times. It happens that the second moment of the resonant eigenmode $\mathrm{He}_4(X)\exp(\frac{1}{2}X^2)$ is zero. Thus Barton's result for the second moment of $h(X)$ is correct when applied to $\tilde{h}(X)$, and furthermore there is no contribution from the logarithmic term. Hence the qualitative conclusion and the quantitative expression for the second moment are both valid.

The second moment of $\bar{c}(z,t)$ is simply the variance. For sufficiently large times we can derive from (12) the asymptotic representation

$$\sigma^2 = 2D_0 t + \text{constant} - \frac{D_2 M^2}{4\pi D_0^2\, 3^{\frac{1}{2}}}t^{-1}+O(t^{-3}\ln t).$$

Except for the error estimate, this confirms Barton's (1976*a*) result. However, if we use the actual solution of (12) and not merely the asymptote, then we can calculate the contribution to the excess variance (i.e. to the constant term) due to buoyancy effects at intermediate times. Indeed, we can interpret the results presented in figure 1 as being an indication of the relative importance of buoyancy effects at short and at intermediate times. Thus, for strongly buoyant narrow discharges, it is *not* justifiable to neglect the short-term effects of buoyancy.

The original derivation of (2) by Erdogan & Chatwin was based upon several physically reasonable (but unjustified) assertions. Barton (1976*b*) concluded that the Erdogan–Chatwin equation correctly described the dominant effect of buoyancy for large Schmidt numbers. He inferred this from the fact that, in the limit of large Schmidt number, the inhomogeneous (i.e. buoyancy) terms in the equation for $C^{(5)}$ were the same for the model equation as they were for the full equations. The two alternative solutions both need to be corrected by the use of 'switchback'. Fortunately, the resonant components of the inhomogeneous terms are necessarily the same in both cases. Thus, when we include the earlier buoyancy term $T^{-5}\ln TC^{(5,1)}$, we find that for large Schmidt numbers both $C^{(5,1)}$ and $C^{(5)}$ are correctly predicted by the Erdogan–Chatwin equation.

6. Smearing-out of a concentration jump

For a discontinuity in concentration the eventual linear solution involves the error function, i.e. the integral of a Gaussian profile. Thus we are led to replace the representation (3) by

$$\bar{c} = c_0 + C(2/\pi)^{\frac{1}{2}} \left[\int_0^{z/\sigma} \exp\left(-\tfrac{1}{2}y^2\right) dy - \sum_{n=1}^{\infty} \frac{b_n(t)}{n!} \mathrm{He}_{n-1}\left(\frac{z}{\sigma}\right) \exp\left\{-\frac{1}{2}\left(\frac{z}{\sigma}\right)^2\right\}\right]. \tag{14}$$

Here c_0 and C are the semi-sum and the semi-difference of the concentrations at plus and minus infinity. If $\sigma(t)$ is chosen to be the exact standard deviation for the concentration gradient $\partial_z \bar{c}$, then $b_2 = 0$ and $b_n(t)$ are precisely the cumulants of $\partial_z \bar{c}$. Indeed, we are in effect solving the nonlinear diffusion equation

$$\partial_t f = \partial_z^2([D_0 + f^2 D_2] f)$$

for $\partial_z \bar{c}$.

As in §2, we use Mehler's formula and the constants $G(i,j,k,n)$ to represent the cubic nonlinearity:

$$(\partial_z \bar{c})^3 = \left(\frac{2C}{\sigma(2\pi)^{\frac{1}{2}}}\right)^3 \sum_{n=0}^{\infty} \left(\sum_{i,j,k} G b_i b_j b_k\right) \mathrm{He}_n\left(\frac{z}{\sigma}\right) \exp\left\{-\frac{1}{2}\left(\frac{z}{\sigma}\right)^2\right\}, \tag{15}$$

where $b_0 = 1$. We observe that the indices of the cumulants are a step removed from those in the analogous representation (5). This means that the most-used constants in the following calculations are

$$G(2m,0,0,0) = (-1)^m/m!\,3^{m+\frac{1}{2}}, \quad G(2m+1,3,0,0) = (-1)^m(m+6)/m!\,2\times 3^{m+\frac{7}{2}}.$$

The resulting sequence of equations, with which we replace the Erdogan–Chatwin equation, is

$$\frac{\sigma^2}{n}\frac{d}{dt}b_n + [b_n + (n-1)b_{n-2}]\frac{1}{2}\frac{d}{dt}\sigma^2$$
$$= (n-1)D_0 b_{n-2} + \frac{2D_2C^2}{\pi\sigma^2}(n-1)! \sum_{i,j,k} G(i,j,k,n-2)\, b_i b_j b_k \tag{16}$$

with $n = 2, 3 \ldots$. There is in addition a minor equation corresponding to $n = 1$:

$$\sigma^2 \frac{d}{dt} b_1 + b_1 \frac{1}{2}\frac{d\sigma^2}{dt} = 0, \quad \text{i.e.} \quad b_1 = \text{constant}/\sigma.$$

A suitable shift of the z axis enables us to set b_1 equal to zero for all time.

The one-term approximation to the $n = 2$ equation for the variance σ^2 is

$$\frac{1}{2}\frac{d\sigma^2}{dt} = D_0 + \frac{2D_2C^2}{\pi\sigma^2}\frac{1}{3^{\frac{1}{2}}}. \tag{17}$$

Again precedence belongs to Prych (1970), though his arguments do not permit a precise evaluation of the nonlinear coefficient. The implicit solution is

$$\sigma^2 - B\ln(\sigma^2 + B) = 2D_0 t + \sigma_I^2 - B\ln(\sigma_I^2 + B)$$

with

$$B = 2D_2C^2/\pi D_0 3^{\frac{1}{2}}.$$

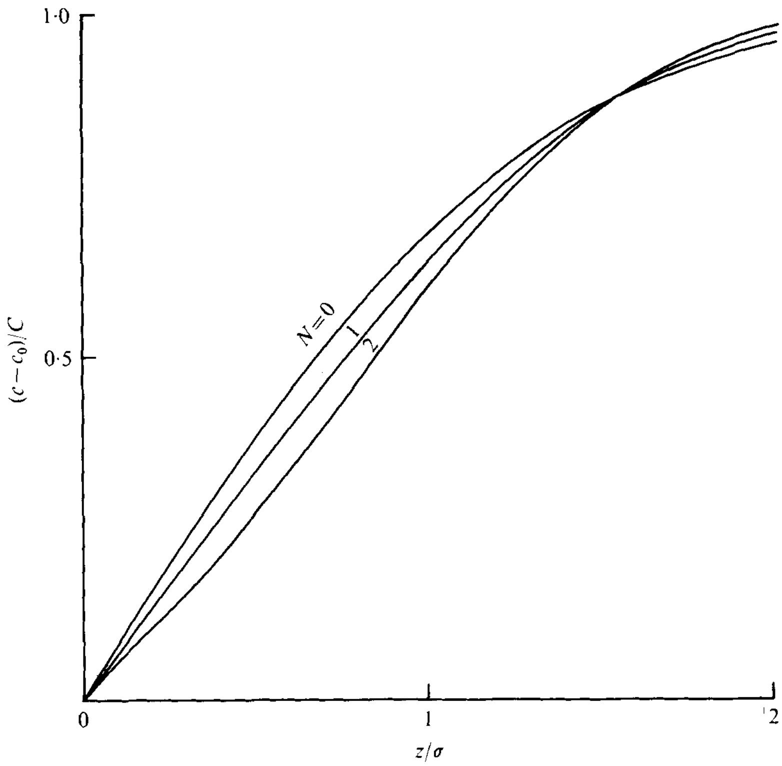

FIGURE 3. Approach to the error-function profile for a concentration jump as the nonlinearity parameter tends to zero.

An important feature of this solution, as was noted by Prych, is that the difference from the linear solution increases indefinitely. Higher-order terms, such as those in (8), (9) and (12) above, merely augment σ^2 by a bounded amount. Thus, in the present case, the simpler model (17) is adequate for most purposes.

One way of interpreting the logarithmic growth of the excess variance is that there is resonance of the $n = 2$ mode (i.e. of the He_1 term). Indeed, in an earlier draft of this paper σ^2 was specified as the linear-theory approximation

$$\sigma^2 = 2D_0(t-t_0)$$

(cf. Barton's papers 1976*a, b*). This led to the explicit occurrence of a logarithmic term in the representation for $\bar{c}$:

$$-C\,\mathrm{sgn}\,(D_2)\,(2/\pi)^{\frac{3}{2}}3^{-\frac{1}{2}}T^{-2}\ln TX\exp\left(-\tfrac{1}{2}X^2\right).$$

Here we take σ^2 to be the exact variance. Thus $b_2 = 0$ and at leading order there is no resonance of any of the even cumulants:

$$b_{2m+2} = N\,\frac{(-1)^m(m+1)(2m+1)!}{mm!\,3^{m+\frac{1}{2}}} + O(N^2\ln|N|).$$

In this context the nonlinearity parameter is defined to be

$$N = 2D_2C^2/\pi D_0\sigma^2.$$

For the odd cumulants the nonlinear forcing terms are only of order σ^{-5} (owing to the absence of b_1). Hence there is resonance only in the b_5 term:

$$b_5 = \beta_3 \left(\frac{2D_2 C^2}{\pi D_0}\right) \frac{28}{3^{\frac{5}{2}}} \sigma^{-5} \ln |N| + \beta_5 \sigma^{-5} + O(\sigma^{-7}),$$

$$b_{2m+1} = \beta_{2m+1} \sigma^{-2m-1} + \beta_3 \left(\frac{2D_2 C^2}{\pi D_0}\right) \frac{(-1)^m (m+6)(2m+1)!}{2^2 (m-2)\, m!\, 3^{m+\frac{3}{2}}} \sigma^{-5} + O(\sigma^{-7} \ln |N|).$$

Retaining only the order-N terms, we find that the concentration distribution is given by

$$\bar{c} = c_0 + C \operatorname{erf}(2^{-\frac{1}{2}} z/\sigma) - C(2/\pi)^{\frac{1}{2}} N \exp\left\{-\frac{1}{2}\left(\frac{z}{\sigma}\right)^2\right\} \sum_{m=1}^{\infty} \frac{(-1)^m}{2m\, m!\, 3^{m+\frac{1}{2}}} \operatorname{He}_{2m+1}\left(\frac{z}{\sigma}\right).$$

Figure 3 shows the profiles of $\bar{c}/C$ for positive values of D_2. Contrary to the results for the approach to normality, in this case the relative steepness increases as the transition region widens. However, as regards the absolute steepness, the resonant contribution to the variance nullifies the importance of this feature. For negative values of D_2 the effects are reversed.

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