# The Discrete Ordinate/Pseudo-spectral Method: Review and Application from a Physicist's Perspective

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#### Abstract

A discussion of the discrete ordinate method for solving differential equations is presented along with a number of examples that have application in various fields of physics. In particular, diffusion cooling, boundary layer meteorology and the diffusion of water in soils are studied. It is shown that the discrete ordinate method is considerably more accurate than finite difference methods of the same order. Results are presented for linear and nonlinear models, with a comprehensive analysis of the results and accuracies.

# 1. Introduction

The discrete ordinate (DO) method appears to have been originally suggested by Wick (1943), but more fully developed by Chandrasekhar (1960) to solve radiative transfer problems. In those early days integral equations were considered, with the integral operator being replaced by a Gaussian quadrature formula and the resulting equation solved at the different quadrature points, along the lines of Williams (1971, Section 11.3.3). Put loosely, the DO method is an analysis of an equation at discrete points in the space under consideration. More precisely, if these points are the roots of a member of a set of orthogonal polynomials, it is simply an orthogonal collocation method. To be consistent with modern-day terminology, we should call it a 'pseudo-spectral method', to which excellent introductions can be found in Gottlieb and Orszag (1977) and Boyd (1989). Whatever the terminology, however, it should be recognised that the method is subsumed by the method of weighted residuals (Finlayson 1972) as pointed out in the review by Robson et al. (1991). The approach yields solutions of differential equations to sometimes stunning accuracy, with far fewer grid points than would be required by comparable finite difference (FD) techniques. In spite of this, it does appear to us that many physicists may be unaware of the tremendous advances that have been made in numerical analysis in recent times. The aim of the present paper then is to wean our colleagues away from the conventional outlook and to illustrate just how powerful and readily accessible the DO/pseudo-spectral method is. (In order to avoid complications, we shall employ the terminology 'DO' in what follows, believing it to be historically correct, but the reader may substitute 'pseudo-spectral' if desired.)

Whereas finite element techniques divide the interval in question into a number of subintervals and approximate the function to be found through low-order, piecewise polynomials, the DO method uses global basis functions of high order, which extend over the entire computational domain. When more accuracy is needed, the finite element technique merely increases the number of subintervals, without varying the degree of the piecewise polynomials. The DO method on the other hand increases the order of the global polynomials, without any subdivision. These remarks apply to both linear and nonlinear systems. Both approaches convert differential or integral equations to algebraic systems: generally speaking, finite element techniques result in large, sparse matrices, whereas the DO method produces low-order, full matrices.

Applications to fluids have been extensive (Canuto *et al.* 1988) up to the scale of global weather phenomena (Haltiner and Williams 1980; Jarraud and Baeda 1986) and the DO method has also been used extensively in kinetic theory by Shizgal and coworkers (Shizgal and Blackmore 1985; Shizgal and Nishigori 1990). Note that in these papers the terminology 'quadrature discretisation method' is used. More comprehensive surveys can be found in Boyd (1989) and Robson *et al.* (1991).

Our fields of study comprise kinetic theory, soil physics and meteorology and the examples we have chosen to illustrate the DO method reflect these interests. However, we have written the paper in a way that we hope will be readily accessible to physicists from all fields, by avoiding specialised jargon, and by presenting our work in a self-contained, practical fashion, rather than through axiomatic development. While we believe that the applications are new, we do not claim that all the discussion on numerical aspects is original or, if it is, then it may raise more questions than it answers!

We briefly review the DO algorithm in Section 2, while Section 3 is devoted to linear eigenvalue problems, derived from pollution meteorology and the kinetic theory of electron swarms. In Section 4 we examine the nonlinear diffusion equation of soil physics. In most cases we confirm the credentials of the DO method by choosing benchmark models, for which analytic solutions are available to test the accuracy of the numerical results. In some cases the accuracy is phenomenal (to machine precision) while in other cases it is entirely unsatisfactory. We also make a number of comparisons with standard finite difference results, which point to the general superiority of the DO method.

#### 2. Discrete Ordinate/Pseudo-spectral Method

Physicists are well aware, from quantum theory, of the importance of obtaining representations of certain operators with respect to some basis. In this section, we prepare the way for solution of differential equations by introducing suitable representations of differential operators in what we might call the DO basis. The algorithm is exact when the function at hand is a polynomial, and therefore it is important to bring to bear whatever physical information/intuition is available to transform the equation to a form where the solution somehow mimics a polynomial.

The essence of the method of weighted residuals and the closely related spectral method is explained in Robson *et al.* (1991, Section 2) and Boyd (1989,

Chapter 1). If f(x) is the function to be found and  $T_i(x)$ , i = 1, ..., N is a set of N 'trial' or 'basis' functions, then we write

$$f(x) \approx \sum_{i=1}^{N} f_i T_i(x) \tag{1}$$

for all x in the interval I under consideration. The expansion coefficients  $f_i$  are determined by some criterion which minimises the error  $\epsilon(x)$  associated with substitution of (1) into the equation to be solved. The discrete ordinate, or pseudo-spectral, method involves choosing the  $T_i(x)$  as interpolating polynomials,

$$T_i(x) \equiv \frac{\phi_N(x)}{(x-x_i)\phi'_N(x_i)},\tag{2}$$

where  $\phi_N(x)$  is an  $N^{\text{th}}$  order polynomial with zeros at  $x_1, \ldots, x_N$ .

In this case, the trial functions have the property

$$T_i(x_j) = \delta_{ij} \tag{3}$$

and the expansion coefficients are

$$f_i = f(x_i) \,. \tag{4}$$

The residual error is forced to vanish at each of the mesh points:  $\epsilon(x_i) = 0$ , i = 1, ..., N. This prescription casts the differential or integral equation into algebraic form, with matrices representing operators. In this paper, we consider only differential equations and therefore we need only the matrix  $D_{ij}$  representing the differential operator

$$\mathcal{D} \equiv \frac{\mathrm{d}}{\mathrm{d}x} \,. \tag{5}$$

Thus from (1) we have

$$\mathcal{D}f|_{x=x_i} \approx \sum_{j=1}^N D_{ij}f_j,$$
 (6)

where

$$D_{ij} \equiv T'_j(x_i) \,. \tag{7}$$

Substitution from (2) yields, for  $i \neq j$ ,

$$D_{ij} = \frac{\phi'_N(x_i)}{(x_i - x_j)\phi'_N(x_j)}$$
  
=  $\frac{1}{x_j - x_i} \prod_{\substack{k=1 \ k \neq i,j}}^N \frac{x_i - x_k}{x_j - x_k},$  (8)

while the diagonal elements are given by

$$D_{ii} = \frac{\phi_N''(x_i)}{2\phi_N'(x_i)} = \sum_{\substack{k=1\\k\neq i}}^N (x_i - x_k)^{-1} \,. \tag{9}$$

The matrix corresponding to *n*th-order differentiation is just the *n*th power of the *D*-matrix defined above, e.g. for n = 2

$$\left. \frac{\mathrm{d}^2 f}{\mathrm{d}x^2} \right|_{x=x_i} \approx \sum_{j=1}^N (D^2)_{ij} f_j \,. \tag{10}$$

Explicit forms for the errors are well known (Robson *et al.* 1991) and we merely point out here that the above formulas are exact if f(x) is a polynomial of degree  $\leq N-1$ . Equations (8) and (9) allow for quick and efficient computation of the differentiation matrix. It (and any powers required) should be computed at the outset and stored for future use.

We now digress for a moment with a few comments on finite difference representations of  $\mathcal{D}$ . Perhaps the most commonly used numerical differentiation algorithms involve the equally spaced abscissae  $x_i$ , i.e. a mesh generated by

$$x_i = x_{i-1} + h \qquad i = 2, \dots, N.$$

If  $f_i$  denote the corresponding ordinates, then one has, for example, the central difference formula

$$(\mathcal{D}f)_{i} = \frac{\mathrm{d}f}{\mathrm{d}x}\Big|_{x=x_{i}}$$
  
=  $\frac{f_{i+1} - f_{i-1}}{2h} + O(h^{2}),$  (11)

or, in general,

$$(\mathcal{D}f)_i = \sum_{j=0}^{N-1} D_{ij} f_j + E_i^{(N)} , \qquad (12)$$

where  $D_{ij}$  denotes the appropriate matrix representation and  $E_i^{(N)}$  is an error term. For the central differencing method,

$$D_{ij} = \frac{1}{2h} (\delta_{j,i+1} - \delta_{j,i-1}) \,. \tag{13}$$

Forward and backward differencing methods have similar representations. There is, however, no need to restrict such an analysis to equally spaced abscissae and, in fact, in many problems in physics it may be highly undesirable to do so. Adaptive methods, for example, concentrate mesh points in regions of rapidly varying f(x). In contrast to (10), the second-order derivative corresponding to the finite difference representation (11) is not the square of the corresponding matrix (13); rather, we have

$$\left. \frac{\mathrm{d}^2 f}{\mathrm{d}x^2} \right|_{x=x_i} \approx \sum_{j=1}^N D_{ij}^{(2)} f_j \,, \tag{14}$$

where

$$D_{ij}^{(2)} = \frac{1}{h^2} (\delta_{j,i+1} - 2\delta_{ij} + \delta_{j,i-1})$$

$$\neq (D^2)_{ij}.$$
(15)

Table 1. Magnitude of extreme derivative operator elements  $D_{ij}$ , with (i, j)indicated

Scheme	Mi	nimum	Maximum		
Uniform Chebychev Legendre	(12,1) (14,1) (8,21)	$1 \cdot 1 \times 10^{-5}$ $1 \cdot 2 \times 10^{-1}$ $6 \cdot 0 \times 10^{-2}$	$(21, 12) \\ (21, 20) \\ (1, 2)$	$\begin{array}{r} 3 \cdot 7 \times 10^5 \\ 2 \cdot 7 \times 10^2 \\ 2 \cdot 6 \times 10^2 \end{array}$	

Note that, whereas the elements (8) and (10) are generally all nonzero, the matrices (13) and (15) are sparse, and special algorithms may be invoked when manipulating them. Another important point is that the matrices of (8) and (9) generally have elements with widely disparate values, as illustrated in Table 1. This table presents the extreme values of  $D_{ij}$  obtained for a mesh of N = 21 points in the interval [0, 1] for nodes uniformly distributed in [0, 1], nodes representing the roots of the Chebychev polynomial  $T_{19}(x)$  plus the end points, and nodes representing the roots of the Legendre polynomial  $P_{19}(x)$  plus the end points, respectively. The disparity generally increases with order N and is a potential source of error when it comes to solving differential equations.

As against these apparent disadvantages, however, it is generally found that, for a given degree of accuracy in the final solution, the required order N associated with the DO method is much lower than the order associated with standard finite difference methods. The trade-off therefore lies between small but full matrices on the one hand and very large, but sparse, matrices on the other. Some quantitative investigations of comparative efficiencies are reported below.

# 3. Some Linear Eigenvalue Problems of Physics

#### 3.1 Sturm-Liouville Problems

In this section we shall be concerned with linear second-order ordinary differential equations of the form

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\frac{\mathrm{d}\phi}{\mathrm{d}x}\right) + [\lambda r(x) + q(x)]\phi = 0, \qquad (16)$$

where p(x), q(x) and  $r(x) \ge 0$  are well behaved functions on the interval  $x \in (a, b)$ , while the allowed values of the constant  $\lambda$  (the eigenvalue) are determined by application of the boundary conditions

$$\alpha_a \phi + \beta_a \phi' = 0, \qquad x = a; \qquad \alpha_b \phi + \beta_b \phi' = 0, \qquad x = b, \quad (17)$$

where  $\alpha_a$ ,  $\alpha_b$ ,  $\beta_a$  and  $\beta_b$  are constants, and/or by requiring the solution  $\phi(x)$  to be well behaved in the interval. Equations (16) and (17) are said to define a Sturm-Liouville problem under certain conditions, and many theorems concerning the solutions are to be found in the literature (Birkhoff and Rota 1962). Many physical problems can be reduced to this form and we examine just two in detail in what follows.

In discrete form on a mesh defined by  $x_1 = a, x_2, \ldots, x_{N-1}, x_N = b$  these equations are represented by

$$\alpha_a \phi_1 + \beta_a \sum_{j=1}^N D_{1j} \phi_j = 0, \qquad (18a)$$

$$\sum_{j=1}^{N} L_{ij} \phi_j = 0 \qquad i = 2, \dots, N-1, \qquad (18b)$$

$$\alpha_b \phi_N + \beta_b \sum_{j=1}^N D_{Nj} \phi_j = 0, \qquad (18c)$$

where

$$L_{ij} \equiv \sum_{k=1}^{N} D_{ik} p_k D_{kj} + (\lambda r_i + q_i) \delta_{ij} , \qquad (19)$$

and where  $\phi_i \equiv \phi(x_i)$ , etc. Equations (18) comprise N homogeneous equations in the N unknowns  $\phi_i$  (i = 1, ..., N). Setting the determinant of coefficients equal to zero furnishes an N<sup>th</sup> order polynomial in  $\lambda$  with the N roots  $\lambda_1, \lambda_2, ..., \lambda_N$ , from which the N eigenfunctions  $\phi_1(x), \phi_2(x), ..., \phi_N(x)$  follow. For the numerical calculations which follow, we have used a standard IMSL eigenvalue/eigenfunction package.

Notice that when boundary conditions are prescribed, the differential equation is discretised only at points interior to the interval: any attempt to discretise (16) at the end points as well leads to redundant equations, inconsistent with the boundary conditions. In what follows we choose  $D_{ij}$  according to the DO representation (8) and (9), and solve the Sturm-Liouville problem for values of the coefficients p, q and r corresponding to certain physical problems.

# 3.2 Boundary Layer Meteorology

We wish to apply the DO method to numerically analyse a problem in boundary layer meteorology, namely turbulent dispersion of pollutants in the atmosphere. The usual picture is one where a point or line source emits pollutant into the atmosphere at a steady rate and this is advected horizontally by wind and dispersed vertically by turbulent action at a rate which is governed by the stability of the atmosphere. Vertical motion is limited by the ground at the lower level and, in the model which we examine here, by an elevated temperature inversion aloft at height l. A discussion of the elementary meteorological factors is given by Seinfeld (1986).

The problem is then to calculate the pollutant concentration as a function of downstream distance and height above the ground. We take a line source and assume that a steady state has been reached. In that case, it is well known (Robson 1983) that the solution of the partial differential equation for turbulent diffusion can be reduced to analysis of the Sturm-Liouville problem

$$\frac{\mathrm{d}}{\mathrm{d}z} \left( K_{\mathrm{V}} \frac{\mathrm{d}\phi}{\mathrm{d}z} \right) + \lambda u \phi = 0 \,, \tag{20}$$

where  $z \in (0, l)$  is the vertical coordinate,  $K_V$  is the (vertical) turbulent diffusion coefficient and u is the (horizontal) wind speed. Boundary conditions are homogeneous (17), with  $\alpha$  being an absorption coefficient and  $\beta$  corresponding to the value of  $K_V$  at the boundary in question. Thus  $\alpha = 0$ ,  $\beta \neq 0$  corresponds to an impenetrable boundary and  $\alpha \neq 0, \beta = 0$  correspond to a perfectly absorbing boundary. Generally speaking, u and  $K_V$  are both functions of z.

Let  $\phi_1(z), \phi_2(z), \ldots$  denote the eigenfunctions of (20) corresponding to the non-zero eigenvalues  $\lambda_1, \lambda_2$ . For impenetrable boundaries there is also a zero eigenvalue  $\lambda_0$  for which  $\phi_0 = 1$  and in this case the expression for the concentration involves a sum over all eigenfunctions  $\phi_n(z)$ , with the modes having  $n \ge 1$  being exponentially damped out at distances greater than  $\lambda_n^{-1}$  downstream from the source (see Robson 1983, equation 15). The lowest nonzero eigenvalue is of special interest, as it determines the asymptotic behaviour of the plume downstream. A variational method has been developed (Robson 1983) explicitly for the purpose of calculating this fundamental eigenvalue. As we shall see, the DO method calculates this quantity extremely accurately.

# 3.2.1 Constant Diffusivity and Wind Speed

Near the earth's surface both  $K_{\rm V}$  and u generally vary markedly with height and any realistic model should reflect this behaviour. In the first instance, however, we choose them to be both constants, equal to unity, for the purposes of establishing the credentials of the DO method and to provide a benchmark model. Thus setting  $K_{\rm V} = 1 = u$  in (20) and taking l = 1 leads to a simple differential equation with eigenfunctions

$$\phi_n = \sin n\pi \qquad n = 1, 2, \dots, \tag{21}$$

in the case where the boundary conditions are

$$\phi_n(0) = 0 = \phi_n(1) \,, \tag{22}$$

and eigenvalues

$$\lambda_n = (n\pi)^2 \,. \tag{23}$$

Table 2. Relative errors  $\delta\lambda_n$ ,  $\delta\phi_n$  in eigenvalues and eigenfunctions respectively, for N = 20 nodes, distributed either uniformly in [0,1] or at the zeros of  $T_{18}(x)$  or  $P_{18}(x)$ , plus the end points

	Relativ	ve errors in eige	Relative errors in eigenfunctions			
n	Uniform	Chebychev	Legendre	Uniform	Chebychev	Legendre
1	$-9 \cdot 9 \times 10^{-11}$	$+5\cdot9 \times 10^{-14}$	$-9 \cdot 2 \times 10^{-15}$	$2 \cdot 4 \times 10^{-10}$	$1 \cdot 2 \times 10^{-15}$	$1.5 \times 10^{-14}$
2	$+5.0 \times 10^{-11}$	$+7.9 \times 10^{-14}$	$-7.9 \times 10^{-14}$	$3 \cdot 9 \times 10^{-11}$	$5.8 \times 10^{-4}$	$9.6 \times 10^{-15}$
3	$+2.7 \times 10^{-11}$	$+4.3 \times 10^{-14}$	$-1.8 \times 10^{-15}$	$6 \cdot 0 \times 10^{-11}$	$3 \cdot 0 \times 10^{-13}$	$2 \cdot 5 \times 10^{-14}$
4	$+2.5 \times 10^{-8}$	$-7.7 \times 10^{-13}$	$-8.9 \times 10^{-15}$	$1 \cdot 9 \times 10^{-8}$	$8 \cdot 2 \times 10^{-4}$	$5.6 \times 10^{-13}$
5	$+1.6 \times 10^{-6}$	$-4.9 \times 10^{-11}$	$-2 \cdot 4 \times 10^{-15}$	$1 \cdot 2 \times 10^{-6}$	$5 \cdot 9 \times 10^{-11}$	$7 \cdot 2 \times 10^{-15}$
6	$-2.9 \times 10^{-4}$	$+7.3 \times 10^{-9}$	$+1.6 \times 10^{-12}$	$1 \cdot 3 \times 10^{-11}$	$3 \cdot 9 \times 10^{-5}$	$1 \cdot 1 \times 10^{-8}$
7	$-3.5 \times 10^{-3}$	$+8.2 \times 10^{-8}$	$-7.3 \times 10^{-10}$	$3 \cdot 2 \times 10^{-3}$	$6 \cdot 3 \times 10^{-6}$	$2.8 \times 10^{-6}$
8	†	$-1.4 \times 10^{-6}$	$+1.1 \times 10^{-7}$	†	$1.8 \times 10^{-3}$	$7 \cdot 6 \times 10^{-6}$
9	†	$-2.5 \times 10^{-5}$	$-5.9 \times 10^{-6}$	†	$1.5 \times 10^{-3}$	$8.7 \times 10^{-5}$
10	†	$+3.9 \times 10^{-4}$	$+1.5 \times 10^{-4}$	<u> </u>	$6 \cdot 8 \times 10^{-3}$	$6 \cdot 0 \times 10^{-4}$

rne i denotes a complex quantit	The	t	denotes	$\mathbf{a}$	complex	quantity
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We also define the relative errors

$$\delta \lambda_n \equiv \left[ \lambda_n (\text{computed}) - \lambda_n (\text{analytic}) \right] / \lambda_n (\text{analytic}) , \qquad (24)$$
$$\delta \phi_n \equiv \left\{ \frac{\int_0^1 [\phi_n(x, \text{computed}) - \phi_n(x, \text{analytic})]^2 \, \mathrm{d}x}{\int_0^1 [\phi_n(x, \text{analytic})]^2 \, \mathrm{d}x} \right\}^{\frac{1}{2}} . \qquad (25)$$

Table 2 shows the relative errors in the first 10 eigenvalues computed using the DO method with N = 20 nodes distributed uniformly in [0, 1], with nodes at the zeros of  $T_{18}(x)$  plus end points, and with nodes at the zeros of  $P_{18}(x)$  plus end points, respectively. Machine precision is  $2 \cdot 2 \times 10^{-16}$ , corresponding to a 53 bit mantissa. We note that the accuracy is extremely high for lower eigenvalues, but rapidly deteriorates for higher modes; there are complex values for uniformly spaced nodes, even though the exact analytic eigenvalues (23) are all real. Also shown in Table 2 are r.m.s. errors in the computed eigenfunctions, which also tend to increase with order n. We have not been able to ascertain why the errors for even n are so large, given that the corresponding eigenvalues are extremely accurate. However, the overall accuracy of Chebychev or Legendre nodes versus

$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	N	n = 1	n=2	n = 3	n = 4	n = 5
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	5 10 15 20	$ \begin{array}{c} -9.8 \times 10^{-3} \\ +3.4 \times 10^{-11} \\ 0.0 \\ -3.2 \times 10^{-15} \end{array} $	$ \begin{array}{c} +5 \cdot 2 \times 10^{-1} \\ -1 \cdot 3 \times 10^{-6} \\ +8 \cdot 4 \times 10^{-15} \\ +8 \cdot 9 \times 10^{-16} \end{array} $	$ \begin{array}{c} +1 \cdot 1 \times 10^{-1} \\ +4 \cdot 2 \times 10^{-4} \\ -1 \cdot 5 \times 10^{-10} \\ +5 \cdot 9 \times 10^{-16} \end{array} $	$ \begin{array}{c} & \dagger \\ -1 \cdot 2 \times 10^{-2} \\ +1 \cdot 5 \times 10^{-7} \\ -1 \cdot 9 \times 10^{-14} \end{array} $	$ \begin{array}{c} \dagger \\ +1 \cdot 2 \times 10^{-1} \\ -1 \cdot 9 \times 10^{-5} \\ +3 \cdot 3 \times 10^{-11} \end{array} $
	25 30 35 40 45	$-2 \cdot 3 \times 10^{-14} -4 \cdot 2 \times 10^{-14} -4 \cdot 5 \times 10^{-14} +2 \cdot 8 \times 10^{-14} -2 \cdot 3 \times 10^{-15} $	$-5 \cdot 7 \times 10^{-15}  -5 \cdot 6 \times 10^{-15}  -1 \cdot 8 \times 10^{-15}  -2 \cdot 3 \times 10^{-14}  +2 \cdot 2 \times 10^{-16}$	$-1 \cdot 6 \times 10^{-15} \\ -3 \cdot 9 \times 10^{-15} \\ -6 \cdot 1 \times 10^{-15} \\ -3 \cdot 2 \times 10^{-15} \\ +5 \cdot 9 \times 10^{-16}$	$\begin{array}{c} -2 \cdot 0 \times 10^{-15} \\ -3 \cdot 1 \times 10^{-15} \\ +2 \cdot 2 \times 10^{-16} \\ -3 \cdot 6 \times 10^{-15} \\ +3 \cdot 3 \times 10^{-15} \end{array}$	$\begin{array}{r} -4 \cdot 3 \times 10^{-16} \\ +1 \cdot 3 \times 10^{-15} \\ +1 \cdot 4 \times 10^{-15} \\ -8 \cdot 5 \times 10^{-16} \\ +5 \cdot 7 \times 10^{-16} \end{array}$

Table 3. Errors in computed eigenvalues  $\lambda_n$  as a function of N The  $\dagger$  denotes a complex quantity

uniform nodes is understandable in terms of the discussion given by Robson et al. (1991, Section 4).

Table 3 shows how the relative errors in the first five computed eigenvalues vary with N. Note the rapid convergence towards machine precision. Legendre nodes were employed in all cases. As explained before, one is often interested in only the first few eigenvalues. Even for N = 10, one obtains  $\lambda_1$  to a few parts in  $10^{10}$  and  $\lambda_2$  to about one part in  $10^6$ . By N = 20 these are effectively determined to machine precision!

Similar remarks apply to the case where

$$\phi_n'(0) = 0 = \phi_n'(1) \,,$$

as reported by Prytz (1989). This model has also been investigated by Nokes  $et \ al.$  (1984), who adopted a series method of solution to (20). For a series of 70 terms, the first seven eigenvalues were found to be correct to five decimal places. Higher eigenvalues, however, required more terms in the series for similar accuracy. Nokes  $et \ al.$  (1984) also found that a shooting method solution of the eigenvalue problem seemed to be less efficient than their power-series method. They also comment on attempts by others to bring to bear standard techniques on the dispersion problem.

Nokes *et al.* (1984) estimated the time taken to generate the first seven eigenvalues to be approximately 3 seconds on a Burroughs 6900 computer. Our machine (an 8 MHz IBM/AT Cleveland 286 clone with 80287 math coprocessor) is quite different and direct comparison of times with Nokes *et al.* (1984) may not be meaningful. Instead, we have opted to compare the DO results with those obtained by applying the centred finite difference formula (15) directly. Table 4 shows the ratio of the computation time using the DO method to that of the FD method for a given order of nodes, N. Clearly, the DO method takes considerably longer than the FD method.

Table 5 shows the relative increase in computational times for the DO and FD methods respectively, as the number of nodes is increased from N = 10 to N = 100. The scaling, as far as eigenvalues are concerned, is roughly  $N^2$  for the FD method and  $N^3$  for the DO method. A detailed breakdown of the times associated with various steps in the respective procedures was given by Prytz (1989). The

N	Eigenvalues	Eigenfunctions
10	$3 \cdot 2$	2.8
20	8.5	$2 \cdot 5$
30	12	$2 \cdot 5$
40	16	$2 \cdot 7$
50	18	$2 \cdot 5$
100	36	$2 \cdot 6$

 Table 4. Relative computational time (s) of DO method with respect to the FD method

Table 5. Relative computational time to solve for N = 100 with respect to N = 10

Method	Eigenvalues	Eigenfunctions
Discrete ordinate	744	862
Finite difference	66	935

telling point in favour of the DO method, however, lies in the accuracy achieved for relatively low *n*. We have seen that for N = 20 nodes consisting of the roots of  $L_{18}(x)$  plus end points, the lowest eigenvalue is calculated to around machine precision,  $10^{-15}$ . For this *N* even the tenth eigenvalue was found to be good to  $2 \times 10^{-3}$ . The time taken to compute all the eigenvalues was  $5 \cdot 72$  s.

On the other hand, for N = 20, for which the FD computation time was 0.67 s, the accuracy of the lowest eigenvalue is just  $2 \times 10^{-3}$ , while for the tenth it is a poor  $2 \times 10^{-1}$ . Increasing N to 100 yields accuracies of  $8 \times 10^{-5}$  and  $8 \times 10^{-3}$  respectively, with a computation time from Table 4 of  $66 \times 0.67 = 44$  s. Accuracy improves as  $1/N^2$  in the FD method, so that even at N = 1000 the accuracies are  $8 \times 10^{-7}$  and  $8 \times 10^{-5}$  respectively. Clearly, an extremely high value of N is needed to get accuracies comparable with the near-machine accuracy that the DO method furnishes using only N = 20 nodes.

The above comparisons should be taken only as a guideline, given that the FD formulas can be refined considerably. However, we do believe that the phenomenal accuracy achievable for the lowest eigenvalues at low N places the DO method virtually in a class of its own, no matter what the level of sophistication of any competitor that might be proposed. The reader can interpret this as a challenge and can readily compare the efficiency of his/her own preferred routine with the DO method, given the simplicity of the formulas (8) and (9) and the ease of implementation of the latter.

# 3.2.2 Constant Wind Speed, Parabolic Diffusivity

The solutions of (20) with u = 1,  $K_V = z(1 - z)$ , which are well behaved throughout the interval (0, 1), are the Legendre polynomials

$$\phi_n = P_n(2z - 1), \qquad (26)$$

with corresponding eigenvalues

$$\lambda_n = n(n+1)$$
  $n = 0, 1, 2, \dots$  (27)

For impenetrable boundaries, the boundary conditions

$$K_{\rm V} \frac{\mathrm{d}\phi_n}{\mathrm{d}z} = 0 \qquad z = 0,1 \tag{28}$$

are automatically satisfied in this case. All we require is that the eigenfunctions be non-singular at z = 0, 1, and in this sense the boundary conditions are 'free'. This constraint is automatically guaranteed when implementing the DO method, which effectively fits a polynomial of degree N - 1 to the N grid points.

Relative errors in the computed eigenvalues  $\lambda_n$  are shown in Table 6 for N = 21, along with r.m.s. errors in the computed eigenfunctions  $\phi_n(z)$ , for various choices of nodes. The extremely high accuracy is not really astonishing in this case, as the analytic solutions are polynomials (26) and the DO algorithm (6) together with (8) and (9) is then supposed to be exact. Of course, one is limited by machine accuracy and round-off errors do propagate, so the entries in Table 6 are not exactly zero, as they ideally should be.

Note that Nokes *et al.* (1984) reported that their series method of solution for 70 terms yielded the first seven eigenvalues accurate to five decimal places in this case, i.e. comparable to the constant wind speed–constant diffusivity case discussed

Table 6. Relative errors in computed eigenvalues and corresponding r.m.s. values for eigenfunctions for the case of constant wind speed and parabolic diffusivity, using the DO method with N = 21 nodes corresponding to (i) uniform distribution; (ii) roots of  $T_{19}(x)$  and 0,1; and (iii) roots of  $P_{19}(x)$  and 0,1

n	Relativ	ve errors in eige	nvalues	Relative	errors in eiger	functions
	Uniform	Chebychev	Legendre	Uniform	Chebychev	Legendre
0	$+8.1 \times 10^{-11}$	$+3\cdot4 \times 10^{-14}$	$-3 \cdot 2 \times 10^{-14}$	$4 \cdot 9 \times 10^{-11}$	$1 \cdot 2 \times 10^{-14}$	$1.8 \times 10^{-14}$
1	$+1.2 \times 10^{-11}$	$-7.3 \times 10^{-14}$	$+1.3 \times 10^{-14}$	$7.5 \times 10^{-12}$	$1.7 \times 10^{-14}$	$8 \cdot 1 \times 10^{-15}$
<b>2</b>	$-3 \cdot 2 \times 10^{-11}$	$-4.0 \times 10^{-14}$	$-5.8 \times 10^{-15}$	$9.8 \times 10^{-11}$	$1.5 \times 10^{-14}$	$6 \cdot 2 \times 10^{-15}$
3	$-5.9 \times 10^{-12}$	$+7.3 \times 10^{-15}$	$-7.4 \times 10^{-16}$	$9 \cdot 9 \times 10^{-12}$	$2 \cdot 5 \times 10^{-14}$	$2.5 \times 10^{-15}$
4	$+1.2 \times 10^{-11}$	$+1.9 \times 10^{-14}$	$+1.8 \times 10^{-15}$	$2 \cdot 9 \times 10^{-11}$	$4 \cdot 2 \times 10^{-14}$	$4.8 \times 10^{-15}$
<b>5</b>	$+3.4 \times 10^{-12}$	$+1.2 \times 10^{-14}$	$-2 \cdot 4 \times 10^{-16}$	$1.5 \times 10^{-11}$	$1 \cdot 1 \times 10^{-14}$	$9.6 \times 10^{-15}$
6	$-4.9 \times 10^{-12}$	$-1.5 \times 10^{-15}$	$-5 \cdot 1 \times 10^{-16}$	$1 \cdot 4 \times 10^{-11}$	$2 \cdot 0 \times 10^{-14}$	$1.7 \times 10^{-15}$
7	$-1.6 \times 10^{-12}$	$-4.6 \times 10^{-15}$	$-2.5 \times 10^{-16}$	$1 \cdot 1 \times 10^{-11}$	$2.7 \times 10^{-14}$	$3 \cdot 2 \times 10^{-15}$
8	$+1.2 \times 10^{-12}$	$+3.9 \times 10^{-16}$	$+2.8 \times 10^{-15}$	$2 \cdot 0 \times 10^{-11}$	$2 \cdot 0 \times 10^{-14}$	$9.3 \times 10^{-14}$
9	$+2.7 \times 10^{-13}$	$+3.2 \times 10^{-15}$	$-7.9 \times 10^{-16}$	$5 \cdot 1 \times 10^{-12}$	$3.3 \times 10^{-13}$	$6.6 \times 10^{-15}$
10	$+4.1 \times 10^{-13}$	$+5.2 \times 10^{-15}$	$-1.3 \times 10^{-15}$	$2 \cdot 6 \times 10^{-12}$	$1.3 \times 10^{-14}$	$5.1 \times 10^{-15}$
11	$+3.8 \times 10^{-13}$	$+3.4 \times 10^{-15}$	$+4.3 \times 10^{-16}$	$1.4 \times 10^{-12}$	$1.2 \times 10^{-14}$	$2.6 \times 10^{-15}$
12	$-6.6 \times 10^{-13}$	0.0	$-5.5 \times 10^{-16}$	$6.5 \times 10^{-12}$	$1 \cdot 2 \times 10^{-14}$	$1.7 \times 10^{-14}$
13	$-4.5 \times 10^{-13}$	$-1 \cdot 1 \times 10^{-15}$	$+6.2 \times 10^{-16}$	$5.2 \times 10^{-12}$	$1.7 \times 10^{-14}$	$6.0 \times 10^{-15}$
14	$+3.8 \times 10^{-13}$	$+2.2 \times 10^{-15}$	$-5.4 \times 10^{-16}$	$3.7 \times 10^{-12}$	$4 \cdot 2 \times 10^{-14}$	$2.1 \times 10^{-14}$
15	$+3.0 \times 10^{-13}$	$+2.7 \times 10^{-15}$	$+2.4 \times 10^{-16}$	$4 \cdot 2 \times 10^{-12}$	$2.5 \times 10^{-14}$	$8.4 \times 10^{-15}$
16	$-1.3 \times 10^{-13}$	$+1.7 \times 10^{-15}$	$+1.7 \times 10^{-15}$	$1.8 \times 10^{-12}$	$7.7 \times 10^{-14}$	$1.0 \times 10^{-14}$
17	$-1.3 \times 10^{-13}$	$-1.5 \times 10^{-14}$	$-5.6 \times 10^{-16}$	$4.5 \times 10^{-13}$	$3.8 \times 10^{-14}$	$4.0 \times 10^{-15}$
18	$+3.0 \times 10^{-14}$	$-1.2 \times 10^{-14}$	$+1.7 \times 10^{-16}$	$4.6 \times 10^{-13}$	$2.6 \times 10^{-14}$	$8.4 \times 10^{-15}$
19	$+2.8 \times 10^{-14}$	$+1.0 \times 10^{-14}$	$-1.0 \times 10^{-15}$	$3.0 \times 10^{-12}$	$5.9 \times 10^{-14}$	$6.7 \times 10^{-15}$
20	$-1 \cdot 2 \times 10^{-14}$	$+6\cdot4 \times 10^{-15}$	$-4 \cdot 1 \times 10^{-16}$	$4 \cdot 4 \times 10^{-14}$	$4 \cdot 0 \times 10^{-14}$	$3.7 \times 10^{-15}$

at length in Section 3.2.1. There is an obvious vast improvement when the DO method is used. We feel that the credentials of the DO method are by now well established through this and the previous model analysis, and we now move on to applications to real problems.

## 3.2.3 Realistic Cases

Meteorological factors control u(z) and  $K_v(z)$  (Seinfeld 1986; Hoffert 1972) which would normally be given as input data in tabulated or parametrised form for the purpose of solving the eigenvalue problem. Such data would, of course, be subject to experimental error, and the question naturally arises as to how much the errors in the coefficients affect the accuracy of the computed eigenvalues and eigenfunctions. We shall address this important aspect of the problem later in Section 3.3 below.

For the present, we shall focus on ways in which one might estimate the error in computed eigenvalues for realistic cases given that we have, of course, no analytical solutions to compare with, in contrast to the previous two simple cases. We take as our example a model based on that of Eschenroeder and Martinez (1970) for the Los Angeles basin:

$$U(z) = 2z \qquad 0 \le z \le 1,$$
  

$$K_{\rm V}(z) = \begin{cases} 0.16 + 2.016z \qquad 0 \le z < 0.417 \\ 1.0 \qquad 0.417 < z < 0.777 \\ 0.16 - 3.78(z - 1) \qquad 0.777 < z \le 1. \end{cases}$$
(29)

The eigenvalue problem was solved for various N with nodes at the roots of Legendre polynomials and impenetrable boundaries  $\phi'_n(0) = 0 = \phi'_n(1)$ . Table 7 shows the first four eigenvalues as calculated by Chappel (1989). Computed eigenvalues converge to the true value in a damped oscillatory fashion (cf. Table 3). The amplitude of the oscillation allows us to put error bars on our estimates of eigenvalues. Thus, for example, from Table 7 we have  $\lambda_1 = 11 \cdot 63 \pm 0 \cdot 02$ ,  $\lambda_2 = 36 \cdot 9 \pm 0 \cdot 1$ , and so on.

Table 7. Eigenvalues for the model (29) for various values of N, as calculated by Chappel (1989)

Ν	10	12	14	18	22	26
$\overline{\lambda_1}$	11.76	$11 \cdot 60$	$11 \cdot 66$	$11 \cdot 60$	$11 \cdot 62$	11.65
$\lambda_2$	$37 \cdot 20$	$36 \cdot 94$	$36 \cdot 97$	$37 \cdot 07$	$36 \cdot 82$	36.88
$\lambda_3$	$79 \cdot 92$	$75 \cdot 81$	$75 \cdot 44$	$76 \cdot 21$	$75 \cdot 59$	$75 \cdot 63$
$\lambda_4$	97.39	$131 \cdot 80$	$131 \cdot 17$	130.09	$130 \cdot 36$	$130 \cdot 64$

Other realistic cases, including the famous logarithmic wind profile, are dealt with in the thesis of Chappel (1989) using the DO method. In accordance with our experience of the model calculations in Sections 3.2.1 and 3.2.2, it is our opinion that the DO method algorithm offers the most efficient way to produce accurate values of the lowest few eigenvalues and, in situations where only asymptotic estimates are needed, that will often suffice. Of course, when the complete concentration profile is needed, summation over many modes n may be required, and then the DO method may lose its distinct advantage.

# 3.3 Kinetic Theory of Gases

We now consider a quite different problem. Here the physical situation corresponds to Cavallieri's experiment (Huxley and Crompton 1974; Rhymes and Crompton 1975) in which electrons created by photoionisation in a cylindrical chamber a few centimetres in dimension diffuse through a gas to conducting walls where they are absorbed. Electron number is determined as a function of time and, asymptotically at long times, is usually observed to decay exponentially with some time constant  $\tau_0$ , which can be interpreted in terms of an effective diffusion coefficient of electrons in the gas occupying the container. Theory shows that this fundamental time constant is inversely proportional to the lowest eigenvalue  $\lambda_0$  of the equation

$$\frac{\mathrm{d}}{\mathrm{d}u} \left( u^2 Q_{\mathrm{m}} \mathrm{e}^{-u} \frac{\mathrm{d}\phi}{\mathrm{d}u} \right) + \kappa^2 \left( \lambda u^{\frac{1}{2}} - \frac{u}{Q_{\mathrm{m}}} \right) \mathrm{e}^{-u} \phi = 0, \qquad (30)$$

which arises in solution of Boltzmann's equation by separation of variables (Leemon and Kumar 1975; Robson 1976). The electron energy distribution consists of a sum over all eigenfunctions  $\phi_n(u)$  (n = 0, 1, 2...), each term being weighted by an exponential damping factor with time constant  $\lambda_n^{-1}$ . At long times, the fundamental mode dominates. The mathematical parallels between this problem and the turbulent dispersion analysed in Section 3.2 above are obvious. In (30),  $u \in (0, \infty)$  denotes the electron energy (scaled to the thermal energy  $k_{\rm B}T$  of the gas atoms),  $Q_{\rm m}$  is the electron-atom momentum-transfer cross section, and  $\kappa$  is a constant geometrical factor determined by the size and shape of the containing vessel. Further details can be found in Robson (1976) and Leemon and Kumar (1975). Equation (30) is to be solved with free boundary conditions, the only constraint put on the solutions being that they are well behaved throughout  $(0, \infty)$ .

There are several interesting physical sidelines to this problem, notably the phenomenon of 'diffusion cooling', whereby the energy dependence of  $Q_{\rm m}(u)$  may provide a 'window' for high-energy electrons to escape to the walls. This is reflected through the existence of an effective diffusion coefficient, which depends upon geometry and gas pressure, and approaches the classical thermal equilibrium coefficient only in the limit of high pressure and/or infinite geometry [ $\kappa \to 0$  in (30)].

Analytic solution of (30) is possible for  $Q_{\rm m} \propto u^{\pm \frac{1}{2}}$  but in general we must seek numerical solutions. Leemon and Kumar (1975) used a polynomial expansion technique, while Robson (1976) developed a variational method, valid also for the case where inelastic collisions occur, to obtain  $\lambda_0$ . It is surprising that no solution of (30) through FD methods has yet been published.

## 3.3.1 A Model Calculation

For a cross section of the form  $Q_{\rm m} = u^{\beta}$ , where  $\beta$  is an arbitrary constant, (30) becomes

$$\frac{\mathrm{d}}{\mathrm{d}u} \left( u^{z+\beta} \mathrm{e}^{-u} \frac{\mathrm{d}\phi}{\mathrm{d}u} \right) + \kappa^2 (\lambda u^{\frac{1}{2}} - u^{1-\beta})\phi = 0.$$
(31)

If  $\beta = -\frac{1}{2}$ , the analytic eigenvalues are (Parker 1965)

$$\lambda_n = \frac{3}{4\kappa^2} (\sqrt{1 + 4\kappa^2 - 1}) + \frac{n}{\kappa^2} \sqrt{1 + 4\kappa^2}, \qquad (32)$$

for n = 0, 1, 2... A typical value of the geometrical constant corresponding to experiment is  $\kappa = 2$ , and in that case

$$\lambda_n = 0.58558 + 1.03078n \,. \tag{33}$$

This provides a benchmark against which we can test the accuracy of computed eigenvalues using the DO algorithm. To do this we take N = 20 nodes corresponding to the zeros of the Laguerre polynomial  $L_{20}(x)$ .

If (31) is solved numerically as it stands, the computed eigenvalues deviate by an unacceptably large factor (>10%) from the exact values (33). (N.B. We must compute  $\lambda_0$  to at least the same level of accuracy as obtained in experiment, namely 1% or better.) It was found that it is important to extract the factor  $u^{\frac{1}{2}}e^{-u}$  from (31), which may then be written in the form

$$\frac{\mathrm{d}}{\mathrm{d}u} \left( u^{\frac{3}{2}+\beta} \frac{\mathrm{d}\phi}{\mathrm{d}u} \right) + (\frac{1}{2}-u) u^{\frac{1}{2}+\beta} \frac{\mathrm{d}\phi}{\mathrm{d}u} + \kappa^2 (\lambda - u^{\frac{1}{2}-\beta}) \phi = 0.$$
(34)

The errors  $\delta \lambda_n$  in the computed eigenvalues of (34) are shown in Table 8 for  $\beta = -\frac{1}{2}$ . Accuracy of the low-*n* eigenvalues lies within acceptable limits, but is

Table 8. Relative errors in eigenvalues of (34) for  $\beta = -\frac{1}{2}$ compared with N = 20 and nodes chosen at the zeros of the Laguerre polynomial using the DO algorithm

$\overline{n}$	$\delta\lambda_n$	n	$\delta\lambda_n$
0	$-2.4 \times 10^{-5}$	5	$3.5 \times 10^{-2}$
1	$-2.5 \times 10^{-4}$	6	$1 \cdot 1 \times 10^{-1}$
<b>2</b>	$-2.0 \times 10^{-3}$	7	$2 \cdot 0 \times 10^{-1}$
3	$-8.0 \times 10^{-3}$	8	$3 \cdot 1 \times 10^{-1}$
4	$-4 \cdot 9 \times 10^{-3}$	9	$4 \cdot 3 \times 10^{-1}$

Table 9. Deviation of computed eigenvalues of (38) from exact analytic values (33)

$\overline{n}$	$\delta\lambda_n$	n	$\delta\lambda_n$	n	$\delta\lambda_n$	n	$\delta\lambda_n$
0	$-2.4 \times 10^{-14}$	5	$-2.9 \times 10^{-12}$	10	$-1.2 \times 10^{-9}$	15	$+4.1 \times 10^{-9}$
1	$+2.5 \times 10^{-15}$	6	$+1.5 \times 10^{-11}$	11	$+3.1 \times 10^{-9}$	16	$-2.0 \times 10^{-9}$
<b>2</b>	$+5.4 \times 10^{-15}$	7	$-4.6 \times 10^{-11}$	12	$-5.4 \times 10^{-9}$	17	$+6.6 \times 10^{-10}$
3	$-8.8 \times 10^{-14}$	8	$+5.1 \times 10^{-11}$	13	$+6.8 \times 10^{-9}$	18	$-1.4 \times 10^{-10}$
4	$+5.2 \times 10^{-13}$	9	$+2.0 \times 10^{-10}$	14	$-6 \cdot 2 \times 10^{-9}$	19	$+1.6 \times 10^{-11}$

still poor when compared with that reported in Sections 3.2.1 and 3.2.2 above, and warrants further investigation.

It is helpful to note that the exact eigenfunctions for this special case are

$$\phi_n(u) = A_n \exp(\alpha u) L_n^{\frac{1}{2}}(u\sqrt{1+4\kappa^2}), \qquad (35)$$

where  $A_n$  is a normalisation constant and

$$\alpha = \frac{1}{2} - \frac{1}{2}\sqrt{1 + 4\kappa^2}$$
(36a)

$$= -1.56155281281....$$
(36b)

Thus, if we make the substitution

$$\phi = \mathrm{e}^{\alpha u} h \tag{37}$$

in (34), we find

$$u\frac{d^{2}h}{du^{2}} + (\frac{3}{2} - u + 2\alpha u)\frac{dh}{du} + (\kappa^{2}\lambda + \frac{3}{2}\alpha)h = 0.$$
 (38)

The errors associated with eigenvalues computed from this equation are very small, as shown in Table 9. In extracting the exponential term from the solution as in (37), we have in effect reduced the unknown function to a polynomial. Since the DO method implicitly assumes that the function that we are seeking is in fact a polynomial (see first paragraph of Section 2), it is hardly surprising that the substitution (37) produces the best results! (In fact, one may wonder why the errors shown in Table 9 are not even smaller still, comparable with machine accuracy; the answer probably lies in propagation of round-off error, but we have not investigated this.)

We have applied fairly stringent tests on the accuracy of our model calculation, requiring that all eigenvalues be accurate to many figures. This is necessary to gain confidence in our technique. In practice, one has neither analytic solutions available for comparison nor the exact value of  $\alpha$  at hand for the important substitution (37). In any case, one is rarely interested in more than the first two or three eigenvalues, which are generally furnished to sufficiently high precision for practical purposes without the substitution (37) (see Table 8).

#### 3.3.2 Errors in Input Data

For the model calculations in the previous sections we have had access to the full machine precision in solving the differential equation. However, what is the situation when the coefficients p, q and/or r of equation (16) are themselves not known exactly? What effect does this have on the solution? For example, in equation (30), the momentum transfer cross section  $Q_{\rm m}$  is typically known to an accuracy of 1% at best, so is there any point in developing a highly refined algorithm to compute eigenvalues to machine precision? Another factor that

must be carefully considered is that calculating the derivatives of a function that contains small but random errors using the DO algorithm can produce enormous errors. Thus, for example, when formulating the DO representation of (30), the derivatives of any empirical  $Q_{\rm m}$  must not be calculated explicitly; rather, the  $Q_{\rm m}$  should be combined with other functions under the differentiation operation.

In order to illustrate these points, we choose an empirical model cross section

$$Q_{\rm m}(u) = Q_{\rm m}^*(u) [1 + A\delta(u)], \qquad (39)$$

where  $\delta(u)$  is random function of u, fluctuating between  $\pm 1$ , and A is an amplitude. The exact cross section is  $Q_{\rm m}^*$ .

We seek to compute eigenvalues of the equation

$$\frac{\mathrm{d}}{\mathrm{d}u}\left(u\nu\frac{\mathrm{d}h}{\mathrm{d}u}\right) + \left[\frac{1}{2} - u(1+\alpha)\right]\nu\frac{\mathrm{d}h}{\mathrm{d}u} + \alpha\frac{\mathrm{d}}{\mathrm{d}u}(u\nu h) \\ + \left\{\left[\alpha(\alpha-1)\nu - \frac{\kappa^2}{\nu}\right]u + \frac{1}{2}\alpha\nu\right\}h + \kappa^2\lambda h = 0, \quad (40)$$

where we have made the substitution (37) in (30) and have defined

$$\nu = u^{\frac{1}{2}} Q_{\rm m}(u). \tag{41}$$

With the model  $Q_{\rm m}^* = u^{-\frac{1}{2}}$  and  $\kappa = 2$ , as in the previous section, we have computed the first few eigenvalues for a range of error amplitudes A. (The 'error' referred to here arises solely from the error in cross section  $Q_{\rm m}$ , and has nothing to do with the numerical error associated with the numerical algorithm.) The deviations  $\Delta \lambda_n$  from the exact values (A = 0) in equation (33) are shown in Table 10.

 Table 10. Effect of statistical errors on eigenvalue accuracy for the same model as Table 9

 The † denotes a complex quantity

A	n = 0	n = 1	n = 2
$ \frac{1 \cdot 0 \times 10^{-4}}{2 \cdot 0 \times 10^{-4}} \\ 5 \cdot 0 \times 10^{-4} \\ 1 \cdot 0 \times 10^{-3} \\ 2 \cdot 0 \times 10^{-3} \\ 5 \cdot 0 \times 10^{-3} \\ 1 \cdot 0 \times 10^{-2} \\ 2 \cdot 0 \times 10^{-2} $	$\begin{array}{r} +9\cdot2\times10^{-5}\\ -4\cdot9\times10^{-6}\\ -2\cdot5\times10^{-5}\\ -4\cdot1\times10^{-5}\\ -1\cdot9\times10^{-4}\\ -3\cdot7\times10^{-4}\\ +1\cdot7\times10^{-3}\\ -9\cdot0\times10^{-3}\end{array}$	$\begin{array}{c} -3 \cdot 9 \times 10^{-4} \\ -3 \cdot 3 \times 10^{-4} \\ -3 \cdot 8 \times 10^{-4} \\ +1 \cdot 7 \times 10^{-3} \\ +6 \cdot 5 \times 10^{-3} \\ +9 \cdot 0 \times 10^{-3} \\ +2 \cdot 8 \times 10^{-2} \\ +3 \cdot 6 \times 10^{-2} \end{array}$	$\begin{array}{r} +1\cdot 4\times 10^{-3} \\ +3\cdot 4\times 10^{-3} \\ +3\cdot 0\times 10^{-3} \\ +7\cdot 0\times 10^{-3} \\ -3\cdot 6\times 10^{-2} \\ -3\cdot 7\times 10^{-2} \\ -8\cdot 0\times 10^{-2} \\ -9\cdot 5\times 10^{-2} \end{array}$
$5 \cdot 0 \times 10^{-2}$	$-1.9 \times 10^{-2}$	$-2.5 \times 10^{-2}$	$-1 \cdot 2 \times 10^{-2} \dagger$

Note that the error in  $\lambda$  is less than the error A in  $Q_m$ . The situation is shown perhaps more clearly in diagrammatic form in Fig. 1. Note also that the errors in  $\lambda_n$  for  $n \geq 1$  exceed A and increase with n. As a final point about experimental errors, we note that experimental error estimates also include sources of systematic errors. In that case we should choose a more conservative



Fig. 1. Errors  $\Delta \lambda_n \equiv \lambda_n (\text{computed}) - \lambda(A=0)$  in the first three eigenvalues as a function of the amplitude of the statistical error in cross section. The solid line has slope 1 and represents an eigenvalue error equal in magnitude to the statistical error in cross section.

value for A, with a corresponding improvement in the confidence of the results obtained from the DO method.

#### 3.3.3 Noble Gases

We now present calculations of the effective diffusion coefficient  $D_{\text{eff}}$  of electrons in Ne, Xe, Kr and Ar gases in the finite enclosure arrangement of the Cavallieri experiment (Huxley and Crompton 1974; Rhymes and Crompton 1975). We solve the Sturm-Liouville problem (30), given cross sections  $Q_{\text{m}}$  in tabulated form, obtained from inversion of various electron swarm experiments (Huxley and Crompton 1974). We obtain the eigenvalues  $\lambda_0, \lambda_1, \lambda_2, \ldots$  using the DO algorithm and identify the effective diffusion coefficient in terms of the lowest of these:

$$N_{\rm gas} D_{\rm eff} \propto \lambda_0 \,,$$
 (42)

where  $N_{\text{gas}}$  is the number density of gas atoms and the constant of proportionality is easily calculated (Robson 1976). We can also find the effective electron temperature from

$$T_{\rm eff} = T_{\rm gas} \int_0^\infty u^{\frac{3}{2}} \phi_0(u) \,\mathrm{d}u \Big/ \int_0^\infty u^{\frac{1}{2}} \phi_0(u) \,\mathrm{d}u \,, \tag{43}$$

where  $T_{\text{gas}}$  is the gas temperature and  $\phi_0$  the eigenfunction corresponding to the lowest eigenvalue. The above expressions apply in an asymptotic sense if and only if there is good separation between  $\lambda_0$  and the next highest eigenvalue  $\lambda_1$ , so that the fundamental mode really does become distinct at long times.

Thus we present results below for  $D_{\text{eff}}$ ,  $T_{\text{eff}}$  and  $\lambda_1/\lambda_0$ , calculated by applying the DO algorithm to (30). It was found that three- or four-figure accuracy was

Gas pressure	$N_{\rm gas}D_{\rm eff}$	$(10^{24} \text{ m}^{-1} \text{ s}^{-1})$	$\lambda_1/\lambda_0$	$T_{\rm eff}$ (K)
(kPa)	LK	DO	-, -	· · · · · · · · · · · · · · · · · · ·
6.67	$6 \cdot 6$	6.87	$1 \cdot 62$	235.7
8.00	$6 \cdot 9$	$7 \cdot 00$	1.88	$253 \cdot 7$
10.67	$7 \cdot 1$	$7 \cdot 11$	$2 \cdot 60$	$271 \cdot 3$
13.33	$7 \cdot 1$	$7 \cdot 16$	3.53.	$279 \cdot 1$
16.00	$7 \cdot 2$	$7 \cdot 19$	$4 \cdot 68$	$283 \cdot 3$
20.00	$7 \cdot 2$	$7 \cdot 21$	$6 \cdot 81$	286.7
$26 \cdot 66$	$7 \cdot 2$	$7 \cdot 22$	$11 \cdot 4$	289.3
100.00		$7 \cdot 24$	149	$292 \cdot 4$

Table 11. Calculations for neon, showing the effective diffusion coefficient computed via the DO algorithm and the polynomial expansion method of Leemon and Kumar (LK) (1975)

readily achievable by taking N = 20 nodes in most cases. In all cases we have taken  $T_{\rm gas} = 293$  K.

#### 3.3.4 Neon

Leemon and Kumar (1975) applied a polynomial expansion method of solution to (30) and used the cross section data set of Robertson (1972). We have used the same cross section (see the tabulation of  $Q_{\rm m}$  versus energy in the Appendix), and extrapolated where necessary at low energies. We chose the nodes to be the zeros of the associated Laguerre polynomial  $L_{20}^{\frac{1}{2}}(x)$ . Results are shown in Table 11. There is significant diffusion cooling ( $T_{\rm eff} < T_{\rm gas}$ ) at lower pressures. At low pressures there is some disagreement with Leemon and Kumar (1975). Moreover, the separation between  $\lambda_1$  and  $\lambda_0$  is not really sufficient to permit the use of asymptotic formulas, based upon the dominance of a single, fundamental exponentially decaying mode.

Gas pressure (kPa)	$N_{ m gas}D_{ m eff}$ (Ness	$(10^{22} \text{ m}^{-1} \text{ s}^{-1})$ DO	$\lambda_1/\lambda_0$	$T_{\rm eff}$ (K)
0.5	7.802	7.818	8.818	$255 \cdot 2$
$1 \cdot 0$	8.837	$8 \cdot 847$	$22 \cdot 66$	$279 \cdot 2$
$1 \cdot 5$	$9 \cdot 158$	$9 \cdot 166$	$43 \cdot 35$	$285 \cdot 9$
$2 \cdot 0$	$9 \cdot 295$	$9 \cdot 302$	70.79	$288 \cdot 6$
$2 \cdot 5$	9.366	9.373	104.7	$290 \cdot 0$
$3 \cdot 0$	$9 \cdot 407$	$9 \cdot 413$	$144 \cdot 6$	$290 \cdot 8$
$5 \cdot 0$	$9 \cdot 470$	$9 \cdot 476$	$342 \cdot 3$	$291 \cdot 9$
10.0	$9 \cdot 498$	$9 \cdot 504$	$980 \cdot 9$	$292 \cdot 4$
$20 \cdot 0$	$9 \cdot 506$	$9 \cdot 512$	3395	$292 \cdot 6$
$50 \cdot 0$	$9 \cdot 508$	$9 \cdot 514$	20262	$292 \cdot 6$

Table 12. Results for electrons in xenon gas

# 3.3.5 Xenon

For xenon we can compare our results with those of Ness (1989) in an earlier, slightly different adaption of the DO algorithm. We have used the same momentum-transfer cross section data set (Ness 1989). This data set is extensive, covering the energy range  $0 \le \epsilon \le 100$  eV, and is sufficient for our purposes as, with T = 293 K,  $0 \le u \le 3000$ . There is therefore no need for any extrapolation, with an associated increase in uncertainty, as was required for neon.

In this case the cross section data set is shown in the Appendix and the nodes were chosen to coincide with the zeros of the Laguerre polynomial  $L_{20}(x)$ . The results are presented in Table 12. There is good separation between  $\lambda_1$  and  $\lambda_0$ over the entire range of pressures shown. However, significant diffusion cooling is evident only at the lowest pressures. Note that there is agreement between Ness and the current study, represented in Table 12, to about three significant figures.

Gas pressure (kPa)	$N_{ m gas} D_{ m eff} \ (10^{23} \ { m m^{-1} \ s^{-1}})$	$\lambda_1/\lambda_0$ $T_{ m eff}$		
0.5	$1 \cdot 546$	4.750	$204 \cdot 6$	
$1 \cdot 0$	$2 \cdot 024$	$8 \cdot 869$	$249 \cdot 1$	
$1 \cdot 5$	$2 \cdot 245$	$14 \cdot 14$	$266 \cdot 8$	
$2 \cdot 0$	$2 \cdot 366$	$20 \cdot 70$	$275 \cdot 7$	
$2 \cdot 5$	$2 \cdot 438$	$28 \cdot 63$	$280 \cdot 1$	
$3 \cdot 0$	$2 \cdot 484$	$37 \cdot 89$	$283 \cdot 8$	
$5 \cdot 0$	$2 \cdot 564$	$87 \cdot 21$	$289 \cdot 0$	
10.0	$2 \cdot 615$	$275 \cdot 4$	$291 \cdot 6$	
$20 \cdot 0$	$2 \cdot 625$	$642 \cdot 3$	$292 \cdot 4$	
$100 \cdot 0^{*}$	$2 \cdot 639$	6974	$292 \cdot 9$	

 Table 13. Results for electrons in krypton gas

\* Convergence at this pressure was achieved only by taking 50 nodes corresponding to the zeros of  $L_{50}(x)$ .

#### 3.3.6 Krypton

The cross section data set is tabulated in the Appendix. Nodes correspond to the zeros of  $L_{20}(x)$ . Results are shown in Table 13. The separation between  $\lambda_1$  and  $\lambda_0$  is sufficient over the range of pressures shown to warrant the use of a single-exponential asymptotic formula, but it appears that diffusion cooling should be noticeable only at lower pressures.

Table 14. Results for electrons in argon gas calculated using the DO algorithm and compared with earlier calculations of Leemon and Kumar (LK) (1975)

Gas pressure	N D	$N_{\rm m} D = (10^{23}  {\rm m}^{-1}  {\rm s}^{-1})$		T = (K)	
(kPa)	LK	DO DO	A1/ A0	$I_{\text{eff}}(\mathbf{R})$	
1.33	9	8.421	2.974	135.7	
$2 \cdot 67$	13	$12 \cdot 80$	$4 \cdot 441$	190.0	
$4 \cdot 00$	16	$15 \cdot 62$	$6 \cdot 132$	217.8	
5.33	18	$17 \cdot 62$	7.997	$234 \cdot 6$	
6.67	19	$19 \cdot 15$	10.02	$245 \cdot 9$	
8.00	20	20.36	$12 \cdot 22$	$253 \cdot 9$	
10.67	22	$22 \cdot 15$	17.09	264.5	
13.33	23	$23 \cdot 40$	$22 \cdot 56$	$271 \cdot 0$	
16.00	<b>24</b>	$24 \cdot 31$	28.51	275.4	
20.00	26	$25 \cdot 29$	37.98	279.8	
26.66	27	26.33	52.72	$284 \cdot 1$	
100		$28 \cdot 54$	327.7	$291 \cdot 2$	
200		28.76	1210	$292 \cdot 6$	
1000*		$29 \cdot 26$	29450	$292 \cdot 9$	

\* Convergence at this pressure was achieved using 50 nodes.

# 3.3.7 Argon

The cross section used here is tabulated in the Appendix. Leemon and Kumar (1975) used a different data set and this could be at least partly responsible for discrepancies with the present results, as presented in Table 14. At the very lowest pressures, the separation between  $\lambda_1$  and  $\lambda_0$  is sufficiently low to place a question mark over the use of the asymptotic formulas. Diffusion cooling persists right through to relatively high pressures.

This completes our examples in kinetic theory and also marks the end of our applications of the DO method to linear differential equations. In the next section, we outline the application of the DO method to a nonlinear differential equation.

# 4. Application to Soil Physics: Solutions of the Nonlinear Diffusion Equation

Water movement in soils is frequently modelled by solutions of Richards' equation (Kirkham and Powers 1972), and computationally efficient algorithms based on FD techniques (Ross 1990) have recently appeared in the literature. Although these procedures are quite satisfactory, the question naturally arises as to whether or not the DO method offers enhanced efficiency and/or accuracy. This question is addressed here in the context of homogeneous soils, where Richards' equation takes the form of a nonlinear diffusion equation.

This is the first time that the DO method has been applied to this problem. Although it is of somewhat greater complexity, one expects certain features of the experience with linear equations to be evident, e.g. the greater efficiency of the DO method for a given order of accuracy (Section 3.2.1). Indeed, the adaptability of the DO/pseudo-spectral method to nonlinear equations is well known (Boyd 1989).

As the topic is not a familiar one to most physicists and, since the problem is quite a different one from the linear systems discussed in Section 3, we devote Section 4.1 below to some preliminary discussion before proceeding to the numerical analysis in Section 4.2.

#### 4.1 Diffusion Equation and its Transformation

## 4.1.1 Diffusion Equation and Boundary Conditions

We consider moisture transport in unsaturated, homogeneous soil of infinite depth, characterised by hydraulic conductivity  $K(\theta)$  and diffusion coefficient  $\mathcal{D}(\theta)$ , both of which are generally strongly dependent upon the volumetric water content  $\theta$ , which in turn depends upon depth z and time t. (For simplicity, we restrict the discussion to situations where only one spatial coordinate, z, enters into the calculation.) We find  $\theta(z, t)$  from solution of the diffusion equation,

$$\partial_t \theta = -\partial_z K + \partial_z (\mathcal{D}\partial_z \theta), \qquad (44)$$

for  $0 \le z < \infty, 0 \le t < \infty$ , together with the initial condition

$$\theta(z,0) = \theta_{\rm I} \tag{45}$$

and the boundary conditions

$$\theta(0,t) = \theta_{\rm S} \qquad t > 0, \tag{46a}$$

$$\theta(\infty, t) = \theta_{\mathrm{I}} \qquad t \ge 0,$$
(46b)

$$[\mathcal{D}\partial_z \theta]_{z \to \infty} = 0 \qquad t \ge 0, \qquad (46c)$$

where  $\theta_{\rm S}$  and  $\theta_{\rm I}$  are constants corresponding to the surface and initial water content respectively. The dependence of K and  $\mathcal{D}$  upon  $\theta$  is assumed given, but is not needed for the present.

## 4.1.2 Generalised Boltzmann Transformation

We then make the so-called Boltzmann transformation to the new variable (Kirkham and Powers 1972)

$$\lambda = zt^{-\frac{1}{2}},\tag{47a}$$

and also define

$$\tau = t^{\frac{1}{2}} \,. \tag{47b}$$

Equation (44) then becomes

$$\frac{1}{2}\tau\partial_{\tau}\theta + \tau K'(\theta)\partial_{\lambda}\theta = \frac{1}{2}\lambda\partial_{\lambda}\theta + \partial_{\lambda}(\mathcal{D}(\theta)\partial_{\lambda}\theta)$$
(48)

which is a generalisation of a well known equation (Kirkham and Powers 1972) for horizontal diffusion, to the extent that the l.h.s. is nonzero in the present situation. Now  $\theta = \theta(\lambda, \tau)$  satisfies

$$\theta(\infty, \tau) = \theta_{\rm I} \,, \tag{49a}$$

$$\theta(0,\tau) = \theta_{\rm S} \,, \tag{49b}$$

$$[\mathcal{D}\partial_{\lambda}\theta]_{\lambda\to\infty} = 0.$$
(49c)

# 4.1.3 Change of Independent Variable

For numerical purposes we follow tradition and consider  $\lambda$  as the dependent variable and  $\theta, \tau$  as the independent coordinates, i.e. we transform from

$$\theta = \theta(\lambda, \tau)$$

to

$$\lambda = \lambda(\theta, \tau) \,, \tag{50}$$

and hence (48) becomes

$$\tau \partial_{\tau} \lambda - 2\tau K'(\theta) + \lambda + 2\partial_{\theta} [\mathcal{D}(\theta)/\partial_{\theta} \lambda] = 0.$$
(51)

This is to be solved subject to

$$\lambda(\theta_{\rm S},\tau) = 0\,,\tag{52a}$$

$$\lambda(\theta_{\rm I},\tau) = \infty \,, \tag{52b}$$

$$[\mathcal{D}(\theta)/\partial_{\theta}\lambda]_{\theta=\theta_{\mathrm{I}}} = 0.$$
(52c)

The final transformation consists of integration of (51) over  $\theta$  from  $\theta_{\rm I}$  to some arbitrary  $\theta \leq \theta_{\rm S}$ . Thus, if we define the new independent variable

$$\sigma(\theta,\tau) \equiv \int_{\theta_{\rm I}}^{\theta} \lambda(\theta,\tau) \,\mathrm{d}\theta\,,\tag{53}$$

then integration of (51) subject to (52c) gives

$$\tau \partial_{\tau} \sigma - 2\tau [K(\theta) - K(\theta_{\rm I})] + \sigma + 2\mathcal{D}(\theta)/\partial_{\theta}^2 \sigma = 0.$$
(54)

Notice that, by virtue of the definition (53), it follows that

$$\sigma(\theta_{\rm I},\tau) \equiv 0 \tag{55a}$$

and, by virtue of (52a) and (53),

$$[\partial_{\theta}\sigma]_{\theta=\theta_{\rm S}} = \lambda(\theta_{\rm S},\tau) = 0.$$
(55b)

Equation (54) is to be solved subject to the boundary conditions (55). The quantity

$$S(\tau) \equiv \sigma(\theta_{\rm S}, \tau) = \int_{\theta_i}^{\theta_{\rm S}} \lambda(\theta, \tau) \,\mathrm{d}\theta \tag{56}$$

has a special significance, as explained below.

## 4.1.4 Horizontal Diffusion

The diffusion equation for horizontal diffusion is obtained from (44) by omitting the first term on the r.h.s. and calling z the horizontal distance. The corresponding transformed equations can then be obtained from Sections 4.1.1 and 4.1.2 through the simple mathematical device of setting either  $\tau$  or K equal to zero and  $\partial_{\tau} = 0$ . In that case  $\lambda, \sigma$  and S are all independent of  $\tau$ , and have the values  $\lambda(\theta, 0)$ ,  $\sigma(\theta, 0)$  and  $S(\theta)$  respectively. Much work has been done for this case (Philip 1960; Kirkham and Powers 1972) and many analytic solutions are available, which we may use as benchmarks for our numerical calculations.

#### 4.1.5 Infiltration, Sorptivity

We define I(t) to be the cumulative volume of water infiltrated into unit horizontal area of soil after time t, and denote the infiltration rate by

$$i(t) = \frac{\mathrm{d}I}{\mathrm{d}t}$$

Thus we have

$$I = \int_0^\infty (\theta - \theta_{\rm I}) \,\mathrm{d}z\,,$$

which, after integration by parts, becomes

$$I = \int_{ heta_{\mathrm{I}}}^{ heta_{\mathrm{S}}} z \,\mathrm{d} heta$$

and transforms according to (47) to

$$I(\tau) = \tau \int_{\theta_1}^{\theta_S} \lambda(\theta, \tau) \,\mathrm{d}\theta \tag{57a}$$

$$\equiv \tau S(\tau) \,, \tag{57b}$$

where the last step follows from (56).

One advantage of transforming the diffusion equation to (54) is now clear: the latter furnishes  $\sigma(\theta, \tau)$ , from which we may obtain S from (56) and hence I from (57) directly, without further integration. Equation (54) also lends itself to a discussion of semi-empirical formulas for I (Philip 1962) but this aspect of the problem is not discussed here.

Finally, we note that for horizontal diffusion the above formulas still apply, but simplify since S is a constant, S(0), and  $I \propto \tau = t^{\frac{1}{2}}$ . The constant S(0) (usually just given the symbol S elsewhere) is conventionally labelled the 'sorptivity' of the soil. For a recent discussion of this property see Bristow and Savage (1987).

## 4.2 Results and Discussion

#### 4.2.1 Horizontal Diffusion

The equation for horizontal water movement can be formally obtained from (54) by taking  $\tau = 0$ , as explained in Section 4.1.4 above. Thus we solve

$$\sigma \partial_{\theta}^2 \sigma + 2\mathcal{D}(\theta) = 0 \tag{58}$$

for  $\sigma(\theta)$ , subject to the boundary conditions (55). These may be discretised on the mesh  $\theta_1, \theta_2, \ldots, \theta_N$ , where  $\theta_1 = \theta_1$  and  $\theta_N = \theta_S$ , according to the prescription of Section 2, i.e. we generate N nonlinear algebraic equations

$$f_i(\sigma_1, \dots, \sigma_N) = 0 \qquad i = 1, \dots, N \tag{59}$$

in the N unknowns  $\sigma_1 = \sigma(\theta_1), \ldots, \sigma_N = \sigma(\theta_N)$ , where

$$f_1 = \sigma_1,$$
  

$$f_i = 2\mathcal{D}_i + \sum_{j=1}^N \sigma_i (D^2)_{ij} \sigma_j \qquad i = 2, \dots, N-1,$$
  

$$f_N = \sum_{j=1}^N D_{Nj} \sigma_j.$$
(60)

These may be solved by the Newton-Raphson iteration technique which, when it converges, does so very rapidly.

We have solved the above problem for  $\theta_{\rm I} = 0, \theta_{\rm S} = 1$  in several of the cases where analytic solutions are easily obtained; these are shown in Table 15. Philip (1960) has given many more. For a uniformly spaced mesh, the agreement of our computed values with the analytic solutions was excellent (seven figures, single precision) with  $N \leq 20$  and a small number of iterations (less than ten in most cases). In view of this high accuracy, we did not feel it necessary to perform a comprehensive set of computations using a non-uniform mesh, although in accordance with the observations in Section 3, some improvement was noticed as nodes were chosen to be the zeros of Chebychev polynomials (Boyd 1989).

Table 15. Some analytic solutions of equation (58) for  $\theta_{\rm I} = 0$ ,  $\theta_{\rm S} = 1$ The constant *a* is arbitrary, whereas K = 0.56714...

	-	
$\mathcal{D}( heta)$	$\sigma( heta)$	$\lambda + \sigma'(\theta)$
$\frac{\frac{1}{2}a\theta^{a}[1-\theta^{a}/(a+1)]}{\frac{1}{2}\sin^{2}(\pi\theta/2)}$ $\frac{1}{2}K^{2}e^{K\theta}(1+\theta-e^{K\theta})$	$egin{array}{l}  heta -  heta^{a+1}/(a+1) \ (2/\pi)\sin(\pi heta/2) \ 1 +  heta - \mathrm{e}^{K heta} \end{array}$	$\frac{1-\theta^a}{\cos(\pi\theta/2)}\\1-K\mathrm{e}^{K\theta}$

This remarkable precision stems from the intrinsic accuracy of the DO method itself, together with the choice of  $\theta$  as the independent variable. As Fig. 2 demonstrates, a uniform spacing  $\theta$  automatically concentrates the  $\lambda$ -values in regions where the gradient  $\partial_{\lambda}\theta$  is largest. This is also the basic idea in the work of Mosher (1985), who gave ideas for other, more sophisticated, modifications



Fig. 2. A qualitative demonstration of choosing equally spaced nodes on the  $\theta$ -axis and the corresponding concentration of nodes on the  $\lambda$ -axis in regions of largest  $\partial_{\lambda}\theta$ . which could further improve the accuracy. On the other hand, the accuracy of the numerical solutions using the FD representations was found to be only a few per cent at best for the same number N of nodes.

#### 4.2.2 Vertical Diffusion

In the case of vertical diffusion, we solve the partial differential equation (54) for  $\sigma(\theta, \tau)$ , with  $\sigma(\theta, 0)$  specified as the solution of (58). We discretise on the mesh  $\theta_1, \ldots, \theta_N$  as in Section 4.1.4 and employ the DO representation for derivatives in  $\theta$ . However, for the 'time' coordinate  $\tau$ , we use the standard backward finite difference formula

$$[\partial_{\tau}\sigma]_{\tau=\tau_n} = \frac{\sigma(\theta,\tau_n) - \sigma(\theta,\tau_{n-1})}{\Delta\tau}, \qquad (61)$$

on a uniform mesh  $\{\tau_n\}$  defined by

$$\tau_{n+1} = \tau_n + \Delta \tau \qquad n = 1, 2, \dots, M - 1,$$

where  $\Delta \tau$  is a constant and  $\tau_1 = 0$ . If we write

$$\sigma_{i,n} \equiv \sigma(\theta_i, \tau_n) \qquad i = 1, \dots, N \quad n = 1, \dots, M,$$

then the discretised form of (54) is

$$\frac{\tau_n}{\Delta \tau} (\sigma_{i,n} - \sigma_{i,n-1}) - 2\tau_n (K_i - K_{\mathrm{I}}) + \sigma_{i,n} + 2\mathcal{D}_i / \sum_{k=1}^N D_{ik}^2 \sigma_{k,n} = 0.$$

If boundary conditions (55) are also approximated in discrete form, then it follows that at the  $n^{\text{th}}$  time step we must solve the N nonlinear algebraic equations

$$f_i(\sigma_{1,n},\ldots,\sigma_{N,n}) = 0 \qquad i = 1,\ldots,N \tag{62}$$

for the N unknowns  $\sigma_{1,n}, \ldots, \sigma_{N,n}$ , where

$$f_{1} = \sigma_{1,n},$$

$$f_{i} = \left[ \left( \frac{\tau_{n}}{\Delta \tau} + 1 \right) \sigma_{i,n} - \tau_{n} \left( \frac{\sigma_{i,n-1}}{\Delta \tau} + 2(K_{i} - K_{I}) \right) \right] \sum_{k=1}^{N} D_{ik}^{2} \sigma_{k,n} + 2\mathcal{D}_{i}$$

$$i = 2, \dots, N - 1,$$

$$f_{N} = \sum_{k=1}^{N} D_{Nk} \sigma_{k,N}.$$
(63)

The implicit formulation in time through the use of (61) means that the time step  $\Delta \tau$  need not be restricted to very small values. The Newton-Raphson method was again used to solve (62). Analytic solutions are generally not possible



Fig. 3. Moisture content as a function of depth in sand 30 minutes and 90 minutes after beginning of penetration, as calculated from the nonlinear diffusion equation (54) using the DO method with N = 20 uniform nodes, as outlined in Section 4.2.2.

in this case and the integrity of the code formulated from the equations above was tested by comparison with that of Ross (1990) for the model

$$K(\theta) = K_{\rm S}(\theta/\theta_{\rm S})^{2b+3}, \qquad \mathcal{D}(\theta) = \mathcal{D}_{\rm S}(\theta/\theta_{\rm S})^{b+2}. \tag{64}$$

Fig. 3 shows the moisture profile in sand (b = 0.65) for two different times. The agreement with Ross (1990) is excellent in this case, even though only a small number  $N \leq 20$  of uniformly spaced nodes was employed. The initial moisture profile used for Fig. 3 was

$$\theta(z,0) = 0 \cdot 1 = \text{constant},$$

and the model hydraulic conductivity and diffusion coefficients (64) have been employed with the following parameters:

$$b = 0.65, \qquad K_{\rm S} = 7.8 \times 10^{-6} \text{ m s}^{-1},$$
  
$$\theta_{\rm S} = 0.3, \qquad \mathcal{D}_{\rm S} = 8.1 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}.$$

Time stepping according to (61) with M = 11 and 21 steps respectively in the 1.5 hour period yielded the same results to within 0.5%. A similar small change was noted when the number of space nodes was increased from N = 20 to 30. On the other hand, FD techniques of this order proved quite unsatisfactory, particularly in the region of the wetting front, and around 150 nodes were needed to get results comparable with those of the DO method. In Fig. 3 FD results with 20 nodes are shown as stars and with 150 nodes as open circles; the DO results are shown as solid circles.

#### 5. Conclusion

We have applied the DO algorithm to linear differential equations arising in the kinetic theory of gases and boundary layer meteorology, and to the nonlinear diffusion equation describing moisture movement in soils. Numerical solutions have been compared with certain benchmark models, for which analytic solutions are available, in order to establish the credentials of the algorithm and the integrity of the code. In many cases involving the computation of eigenvalues, it was found that, while the lowest eigenvalues were computed to very high accuracy, higher members of the spectrum were subject to larger errors.

For many types of physical problems, however, where only asymptotic regions of space or time are important, it is just the lowest eigenvalue which needs to be found, and hence the DO method is admirably suited to these cases. Comparison with standard FD methods showed that, while these were considerably faster, the solutions are not anywhere near as accurate as those provided by the DO method. Unless limited accuracy is acceptable and speed is paramount, our feeling is therefore that the DO algorithm should be a serious contender in any calculation. The other advantage offered by the DO algorithm lies in its flexibility regarding disposition of nodes, but we did not explore this aspect to any great extent in the present paper.

Finally, as we remarked in the Introduction, the aim of the present paper has been to persuade physicists to consider implementing the DO algorithm to solve differential equations arising in their calculations. We have to report one 'conversion' in the course of writing this paper, to the quantum close-coupling calculation of scattering of rare gas atoms (Leo 1992, personal communication), involving four linear coupled differential equations.

#### Acknowledgments

The support of the James Cook University-CSIRO Collaborative Fund is gratefully acknowledged. One of the authors (R. E. Robson) thanks the Davies Laboratories for their hospitality. We thank Dr Keith Bristow and Dr Peter Ross for constructive discussions and comments during the preparation of this manuscript. We also thank Dr Kevin Ness for useful discussions and for making available preliminary results of his own calculations for comparison in Section 3.3. Prof. R. W. Crompton kindly provided the argon cross sections used in Section 3.3. Our thanks go to him also for his continual encouragement of this work.

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#### Appendix: Cross Section Tables

Here we list tables of the momentum-transfer cross sections used to estimate the effect of diffusion cooling in the noble gases using the DO method. The tables are organised into pairs of columns; the first column of a pair represents the electron energy (in eV) at which a cross section value is given, and the second column the cross section in units of  $Q_0$  (=  $10^{-20}$  m<sup>2</sup>).

# Neon

Neon cross sections were obtained from Robertson (1972). However, since these data are only available for  $\epsilon \geq 0.03$  eV, we have extrapolated the cross sections below 0.03 eV, by fitting a straight line to the first four points, using a log-log transformation. Table 16 lists the momentum-transfer cross sections for neon. Those entries with a  $\dagger$  represent the extrapolated values. (The mass of a neon atom is 20.179 amu.)

$\epsilon$ (eV)	$(10^{-20} \mathrm{m}^2)$	$\epsilon (eV)$	$(10^{-20} \mathrm{m}^2)$	$\stackrel{\epsilon}{(\mathrm{eV})}$	$(10^{-20} \mathrm{m^2})$
0.001	$0.172^{+}$	$0 \cdot 025$	$0.450^{+}$	0.50	1.321
0.002	$0.211^{+}$	$0 \cdot 028$	$0.460^{+}$	0.60	$1 \cdot 402$
0.003	$0.237^{+}$	$0 \cdot 03$	0.469	0.70	$1 \cdot 472$
0.004	$0.258^{+}$	$0 \cdot 04$	0.504	0.80	1.528
0.005	$0.276^{+}$	0.05	0.536	0.90	1.580
0.006	$0.291^{+}$	0.06	0.566	$1 \cdot 00$	$1 \cdot 619$
0.007	$0.305^{+}$	$0 \cdot 07$	0.601	$1 \cdot 20$	1.685
0.008	$0.317^{+}$	0.08	0.636	$1 \cdot 50$	1.753
0.009	$0.329^{+}$	0.09	0.669	$1 \cdot 80$	1.793
0.010	$0.339^{+}$	$0 \cdot 10$	0.701	$2 \cdot 00$	$1 \cdot 815$
$0 \cdot 012$	$0.358^{+}$	$0 \cdot 12$	0.754	$2 \cdot 50$	$1 \cdot 860$
0.014	$0.374^{+}$	0.15	0.828	$3 \cdot 00$	1.906
0.016	$0.390^{+}$	0.18	0.893	$4 \cdot 00$	$1 \cdot 984$
0.018	$0.403^{+}$	$0 \cdot 20$	0.930	$5 \cdot 00$	$2 \cdot 070$
0.020	$0.416^{+}$	$0 \cdot 25$	$1 \cdot 018$	$6 \cdot 00$	$2 \cdot 144$
$0 \cdot 022$	$0.428^{+}$	0.30	$1 \cdot 091$	$7 \cdot 00$	$2 \cdot 213$
$0 \cdot 024$	$0.439^{++}$	$0 \cdot 40$	$1 \cdot 225$		

Table 16. Neon: Momentum-transfer cross sections

Table 17. Xenon: Momentum-transfer cross sections

$\stackrel{\epsilon}{(\mathrm{eV})}$	$(10^{-20} \mathrm{m}^2)$	$\epsilon \ ({ m eV})$	$(10^{-20} \mathrm{m^2})$	$\epsilon$ (eV)	$(10^{-20} \mathrm{m}^2)$	$\stackrel{\epsilon}{(\mathrm{eV})}$	$(10^{-20} \mathrm{m}^2)$
0.000	130.5	0.240	$5 \cdot 453$	0.840	1.175	$3 \cdot 40$	19.70
0.001	$116 \cdot 3$	0.260	$4 \cdot 603$	0.860	$1 \cdot 240$	$3 \cdot 60$	$21 \cdot 40$
0.002	$110 \cdot 0$	0.280	$3 \cdot 908$	0.880	$1 \cdot 300$	$3 \cdot 80$	$22 \cdot 90$
0.003	$105 \cdot 2$	0.300	3.337	0.900	$1 \cdot 370$	$4 \cdot 00$	$24 \cdot 10$
0.005	$97 \cdot 64$	0.320	$2 \cdot 866$	0.920	$1 \cdot 440$	$4 \cdot 20$	$25 \cdot 20$
0.007	$91 \cdot 61$	0.340	$2 \cdot 477$	0.940	$1 \cdot 500$	$4 \cdot 40$	$26 \cdot 20$
$0 \cdot 010$	$84 \cdot 25$	0.360	$2 \cdot 154$	0.960	1.570	$4 \cdot 60$	$27 \cdot 00$
0.015	74.67	0.380	$1 \cdot 885$	0.980	$1 \cdot 640$	$4 \cdot 80$	$27 \cdot 60$
$0 \cdot 020$	$67 \cdot 14$	$0 \cdot 400$	1.661	$1 \cdot 00$	1.720	$5 \cdot 00$	$28 \cdot 20$
$0 \cdot 025$	$60 \cdot 94$	$0 \cdot 420$	$1 \cdot 474$	$1 \cdot 05$	$1 \cdot 910$	$5 \cdot 20$	$28 \cdot 70$
0.030	55.71	$0 \cdot 440$	$1 \cdot 318$	$1 \cdot 10$	$2 \cdot 120$	$5 \cdot 40$	$29 \cdot 00$
$0 \cdot 035$	$51 \cdot 19$	$0 \cdot 460$	$1 \cdot 189$	$1 \cdot 15$	$2 \cdot 330$	$5 \cdot 60$	$29 \cdot 20$
$0 \cdot 040$	$47 \cdot 24$	0.480	$1 \cdot 081$	$1 \cdot 20$	$2 \cdot 550$	$5 \cdot 80$	$29 \cdot 40$
0.050	40.65	0.500	0.9928	$1 \cdot 25$	$2 \cdot 780$	$6 \cdot 00$	$29 \cdot 50$
0.060	$35 \cdot 33$	0.520	0.9208	$1 \cdot 30$	$3 \cdot 030$	$6 \cdot 20$	$29 \cdot 60$
0.070	30.96	0.540	0.8634	$1 \cdot 35$	$3 \cdot 270$	6.60	$29 \cdot 50$
0.080	$27 \cdot 29$	0.560	0.8191	$1 \cdot 40$	$3 \cdot 530$	7.00	$29 \cdot 20$
0.090	$24 \cdot 19$	0.580	0.7866	$1 \cdot 50$	$4 \cdot 080$	7.50	$28 \cdot 60$
$0 \cdot 100$	$21 \cdot 53$	0.600	0.7652	$1 \cdot 60$	$4 \cdot 680$	$8 \cdot 00$	$27 \cdot 70$
0.110	$19 \cdot 23$	0.620	0.7541	1.70	$5 \cdot 320$	8.50	$26 \cdot 50$
0.120	$17 \cdot 24$	0.640	0.7530	$1 \cdot 80$	5.980	9.00	$25 \cdot 00$
$0 \cdot 130$	$15 \cdot 49$	0.660	0.7615	$1 \cdot 90$	6.770	9.50	$23 \cdot 50$
0.140	$13 \cdot 96$	0.680	0.7795	$2 \cdot 00$	7.390	$10 \cdot 0$	$21 \cdot 80$
0.150	$12 \cdot 60$	0.700	0.8069	$2 \cdot 20$	8.950	$11 \cdot 0$	18.50
0.160	$11 \cdot 40$	0.720	0.8437	$2 \cdot 40$	10.60	$12 \cdot 0$	15.50
$0 \cdot 170$	10.34	0.740	0.8899	$2 \cdot 60$	$12 \cdot 40$	$14 \cdot 0$	10.70
0.180	$9 \cdot 392$	0.760	0.9456	$2 \cdot 80$	$14 \cdot 30$	$16 \cdot 0$	8.800
0.190	$8 \cdot 545$	0.780	$1 \cdot 005$	$3 \cdot 00$	$16 \cdot 10$	$18 \cdot 0$	6.500
$0 \cdot 200$	7.787	0.800	$1 \cdot 055$	$3 \cdot 20$	$18 \cdot 00$	$20 \cdot 0$	5.000
$0 \cdot 220$	$6 \cdot 497$	$0 \cdot 820$	$1 \cdot 115$	$3 \cdot 30$	$18 \cdot 80$	100	$1 \cdot 360$

$\frac{\epsilon}{(eV)}$	$(10^{-20} \mathrm{m^2})$	$\stackrel{\epsilon}{(\mathrm{eV})}$	$(10^{-20} \mathrm{m}^2)$	$\epsilon (eV)$	$(10^{-20} \mathrm{m^2})$	$\epsilon (eV)$	$(10^{-20} \mathrm{m}^2)$
$ \begin{array}{c} 0.0\\ 0.05\\ 0.10\\ 0.15\\ 0.20\\ 0.25\\ 0.30 \end{array} $	$\begin{array}{c} 40 \cdot 376 \\ 13 \cdot 288 \\ 7 \cdot 109 \\ 4 \cdot 054 \\ 2 \cdot 349 \\ 1 \cdot 352 \\ 0 \cdot 7637 \end{array}$	$ \begin{array}{c} 0.75 \\ 0.80 \\ 0.85 \\ 0.90 \\ 0.95 \\ 1.00 \\ 1.10 \\ \end{array} $	$\begin{array}{c} 0 \cdot 3099 \\ 0 \cdot 3649 \\ 0 \cdot 4202 \\ 0 \cdot 4737 \\ 0 \cdot 5539 \\ 0 \cdot 6665 \\ 0 \cdot 8020 \end{array}$	$   \begin{array}{r}     1 \cdot 80 \\     1 \cdot 90 \\     2 \cdot 00 \\     2 \cdot 20 \\     2 \cdot 50 \\     2 \cdot 50 \\     2 \cdot 80 \\     2 \cdot 80 \\   \end{array} $	$ \begin{array}{r} 2 \cdot 58 \\ 2 \cdot 84 \\ 3 \cdot 11 \\ 3 \cdot 68 \\ 4 \cdot 56 \\ 5 \cdot 66 \\ 5 \cdot 66 \\ 2 \cdot 82 \\ \end{array} $	$     \begin{array}{r}       8 \cdot 00 \\       9 \cdot 00 \\       10 \cdot 00 \\       11 \cdot 00 \\       12 \cdot 00 \\       13 \cdot 00 \\       \hline       3 \cdot 00   \end{array} $	20.0021.0021.0021.0020.919.4
$\begin{array}{c} 0.30 \\ 0.35 \\ 0.40 \\ 0.45 \\ 0.50 \\ 0.55 \\ 0.60 \\ 0.65 \\ 0.70 \end{array}$	$\begin{array}{c} 0.7637\\ 0.4228\\ 0.2364\\ 0.1468\\ 0.1182\\ 0.1273\\ 0.1589\\ 0.2038\\ 0.2551\end{array}$	$ \begin{array}{c} 1 \cdot 10 \\ 1 \cdot 15 \\ 1 \cdot 20 \\ 1 \cdot 25 \\ 1 \cdot 30 \\ 1 \cdot 40 \\ 1 \cdot 50 \\ 1 \cdot 60 \\ 1 \cdot 70 \\ \end{array} $	$\begin{array}{c} 0.8920\\ 0.9960\\ 1.111\\ 1.215\\ 1.330\\ 1.570\\ 1.810\\ 2.060\\ 2.320\end{array}$	$3 \cdot 00$ $3 \cdot 30$ $3 \cdot 60$ $4 \cdot 00$ $4 \cdot 40$ $4 \cdot 80$ $5 \cdot 00$ $6 \cdot 00$ $7 \cdot 00$	$6 \cdot 30$ $7 \cdot 37$ $8 \cdot 48$ $9 \cdot 92$ $11 \cdot 10$ $12 \cdot 60$ $13 \cdot 20$ $16 \cdot 40$ $18 \cdot 40$	$ \begin{array}{r} 14 \cdot 00 \\ 15 \cdot 00 \\ 16 \cdot 00 \\ 17 \cdot 00 \\ 18 \cdot 00 \\ 19 \cdot 00 \\ 20 \cdot 00 \\ 25 \cdot 00 \\ \end{array} $	$     \begin{array}{r}       17 \cdot 8 \\       15 \cdot 2 \\       14 \cdot 8 \\       13 \cdot 6 \\       12 \cdot 5 \\       11 \cdot 7 \\       11 \cdot 0 \\       8 \cdot 0 \\     \end{array} $

Table 18. Krypton: Momentum-transfer cross sections

Table 19. Argon: Momentum-transfer cross sections

				and the second			
$\epsilon$ (eV)	$(10^{-20} \mathrm{m^2})$	$\epsilon (eV)$	$(10^{-20} \mathrm{m^2})$	$\stackrel{\epsilon}{(\mathrm{eV})}$	$(10^{-20} \mathrm{m^2})$	$\epsilon \ ({ m eV})$	$(10^{-20} \mathrm{m}^2)$
0.0000	7.817	0.028	$2 \cdot 659$	0.28	0.1169	0.88	1.230
0.0001	$7 \cdot 421$	0.030	$2 \cdot 538$	0.30	0.1418	0.90	$1 \cdot 264$
0.0002	$7 \cdot 259$	0.032	$2 \cdot 425$	0.32	0.1715	0.92	$1 \cdot 299$
0.0003	$7 \cdot 136$	0.035	$2 \cdot 268$	$0 \cdot 34$	0.2049	0.94	1.334
0.0004	7.033	0.040	$2 \cdot 035$	0.36	0.2410	0.96	1.370
0.0005	$6 \cdot 942$	0.045	1.831	0.38	0.2791	0.98	1.405
0.0006	$6 \cdot 861$	0.050	1.652	$0 \cdot 40$	0.3187	$1 \cdot 00$	1.441
0.0007	6.787	0.055	$1 \cdot 493$	$0 \cdot 42$	0.3591	$1\cdot 2$	1.66
0.0008	6.718	0.060	1.352	$0 \cdot 44$	0.4002	1.35	1.86
0.0009	$6 \cdot 654$	0.065	$1 \cdot 225$	0.46	0.4414	1.5	2.05
0.0010	6.593	0.070	1.111	0.48	0.4828	$1 \cdot 6$	$2 \cdot 19$
0.0012	$6 \cdot 481$	0.075	$1 \cdot 009$	0.50	0.5240	$1 \cdot 7$	2.33
0.0015	$6 \cdot 332$	0.080	0.9157	0.52	0.5649	$1 \cdot 85$	$2 \cdot 51$
0.0020	$6 \cdot 115$	0.085	0.8317	$0 \cdot 54$	0.6054	$2 \cdot 0$	$2 \cdot 70$
0.0030	$5 \cdot 762$	0.090	0.7555	0.56	0.6455	$2 \cdot 5$	$3 \cdot 43$
0.0040	$5 \cdot 474$	0.095	0.6863	0.58	0.6852	$3 \cdot 0$	$4 \cdot 20$
0.0050	$5 \cdot 228$	0.100	0.6233	0.60	0.7243	$3 \cdot 5$	4.95
0.0060	$5 \cdot 011$	0.110	0.5140	0.62	0.7629	$4 \cdot 0$	5.70
0.0070	$4 \cdot 817$	0.120	0.4236	0.64	0.8010	$5 \cdot 0$	7.4
0.0080	$4 \cdot 640$	0.130	0.3488	0.66	0.8389	6.0	$9\cdot 2$
0.0090	$4 \cdot 478$	$0 \cdot 140$	0.2872	0.68	0.8757	8.0	11.0
0.0100	$4 \cdot 328$	0.150	0.2368	0.70	0.9123	10.0	13.0
0.0120	$4 \cdot 058$	0.160	0.1959	0.72	0.9486	$12 \cdot 0$	14.0
0.0140	$3 \cdot 820$	0.170	0.1633	0.74	0.9845	$14 \cdot 0$	15.0
0.0160	$3 \cdot 607$	0.180	0.1377	0.76	$1 \cdot 0200$	$16 \cdot 0$	14.0
0.0180	$3 \cdot 414$	0.190	0.1183	0.78	1.0553	$20 \cdot 0$	10.0
0.0200	$3 \cdot 238$	$0 \cdot 200$	0.1041	0.80	1.0903	40.0	9.0
$0 \cdot 220$	$3 \cdot 076$	$0 \cdot 220$	0.08916	0.82	$1 \cdot 1252$	60.0	8.0
$0 \cdot 0240$	$2 \cdot 926$	$0 \cdot 240$	0.08838	0.84	$1 \cdot 1600$	80.0	$7 \cdot 0$
0.0260	$2 \cdot 788$	$0 \cdot 260$	0.09847	0.86	$1 \cdot 1958$	100	6.0

## X enon

Xenon cross sections were obtained from Ness (1989). These data are quite extensive, covering the energy range  $0 \le \epsilon \le 100$  eV, sufficient for our analysis as, with T = 293 K,  $0 \le u \le 3000$ . There is therefore no need for any extrapolation, with a subsequent increase in uncertainty, as was required for neon. Table 17 contains the momentum-transfer cross sections for xenon. (The mass of a xenon atom is  $131 \cdot 30$  amu.)

## Krypton

Krypton cross sections were obtained from Elford (1989). These data are also very extensive, covering the energy range  $0 \le \epsilon \le 25$  eV, sufficient for our analysis as, with T = 293 K,  $0 \le u \le 800$ . The estimated error is  $\pm 4\%$  for the range  $0.04 \le \epsilon \le 6.0$  eV. (The mass of a krypton atom is 83.80 amu.)

## Argon

Argon cross sections were obtained from the data file supplied by Crompton (1989, personal communication). These data are extremely detailed, with momentum-transfer cross sections supplied in the range  $0 \le \epsilon \le 10^7$  eV. Below  $2 \times 10^{-3}$  eV, cross sections are listed in  $10^{-4}$  eV steps, to 1 eV in steps of  $10^{-3}$  eV, with various intervals up to  $10^7$  eV. No estimated error range was supplied. (The mass of an argon atom is 39.948 amu.) Table 19 contains only a subset of the complete momentum-transfer cross section data set, as the original data set is too large to reproduce here.

Manuscript received 19 January, accepted 21 June 1993

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