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Note

Use of Implicit and Explicit Flux-Corrected Transport Algorithms in Gas Discharge Problems Involving Non-uniform Velocity Fields

1. Introduction

In many applications of numerical methods to gas discharge theory, the electric field changes rapidly with position [1, 2]. Therefore it is essential to solve the continuity equations for the electrons and ions accurately because space-charge effects dominate the electric fields, and hence the velocity distribution in the gas. Although transport algorithms are often used in such cases they are seldom tested for accuracy in the presence of a spatially varying velocity field. In the cases where such a test has been attempted, an exact solution has not been used for quantitative comparison [3, 4]. In this paper we present the exact solution for the case of a velocity field varying linearly with distance, which can be used to test the accuracy of any algorithm.

The basic equation we wish to solve is

$$\frac{\partial \rho}{\partial t} + \frac{\partial (w\rho)}{\partial x} = 0, \tag{1}$$

where ρ is density, w is the drift velocity, x is position and t is time. A critical parameter in the solution of this equation is the Courant number $c = \delta t \cdot w/\delta x$, where δt is the time step and δx the mesh space.

The algorithms tested are the explicit Phoenical LPE SHASTA algorithm [5] and a newly developed implicit FCT algorithm using a fourth-order scheme [6]. For Courant number $c > 1$ the fourth-order scheme employs a marching method [6], while for $c \leqslant 1$ a tri-diagonal matrix of coefficients is solved.

For a numerical test we use both square and semi-circular wave-forms [6] propagating in the presence of a velocity field that varies linearly with distance. The changes in the shapes of the wave-forms obtained by using two representative FCT algorithms are compared with the analytic solution obtained by the method of characteristics.

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2. Description of Methods

The Phoenical LPE SHASTA method [5] is an explicit method which gives non-negative results only for $c \leqslant 0.5$ in the presence of a non-uniform velocity field. We use the form of the LPE SHASTA algorithm described in detail by Morrow and Cram [4].

In a recent paper [6] we presented a fourth-order space- and time-centered scheme which was used as the high-order scheme for an FCT algorithm. The fourth-order scheme has the following form with a uniform mesh in a non-uniform velocity field,

$$\begin{aligned}(2-3c_{j-1/2}+c_{j-1/2}^2)\,\bar{\rho}_{j-1}&+(8+3c_{j+1/2}-3c_{j-1/2}-c_{j+1/2}^2-c_{j-1/2}^2)\,\bar{\rho}_j\\&+(2+3c_{j+1/2}+c_{j+1/2}^2)\,\bar{\rho}_{j+1}\\&=(2+3c_{j-1/2}+c_{j-1/2}^2)\,\rho_{j-1}^n+(8-3c_{j+1/2}+3c_{j-1/2}-c_{j+1/2}^2-c_{j-1/2}^2)\,\rho_j^n\\&+(2-3c_{j+1/2}+c_{j+1/2}^2)\,\rho_{j+1}^n,\end{aligned} \tag{2}$$

where $c_{j+1/2}=\delta t w_{j+1/2}/\delta x$, $w_{j+1/2}$ is the velocity at the cell boundary between mesh points j and $j+1$, δt is the time step, δx is the mesh space, $\bar{\rho}_j$ is the high-order solution at time level n + 1 and mesh point j, and ρ_j^n is the solution at time level n at mesh point j.

From Eq. (2) we can derive the high-order flux

$$\begin{aligned}\phi_{j+1/2}^H=&\frac{(2+c_{j+1/2}^2)}{12}(\bar{\rho}_{j+1}-\bar{\rho}_j-\rho_{j+1}^n+\rho_j^n)\\&+\frac{c_{j+1/2}}{4}(\bar{\rho}_{j+1}+\bar{\rho}_j+\rho_{j+1}^n+\rho_j^n).\end{aligned} \tag{3}$$

For non-uniform positive velocities we can use upwind difference for the low-order solution

$$\tilde{\rho}_j=\rho_j^n-c_{j+1/2}\rho_j^n+c_{j-1/2}\rho_{j-1}^n, \tag{4}$$

where $\tilde{\rho}_j$ is the low-order solution at time level $n+1$ and mesh point j.

Thus the low-order flux is

$$\phi_{j+1/2}^L=c_{j+1/2}\rho_j^n \tag{5}$$

and the anti-diffusive flux is then

$$\begin{aligned}\phi_{j+1/2}=&\frac{(2+c_{j+1/2}^2)}{12}(\bar{\rho}_{j+1}-\bar{\rho}_j-\rho_{j+1}^n+\rho_j^n)\\&+\frac{c_{j+1/2}}{4}(\bar{\rho}_{j+1}+\bar{\rho}_j+\rho_{j+1}^n-3\rho_j^n).\end{aligned} \tag{6}$$

Equation (2) can be solved as a tri-diagonal matrix for $c \leqslant 1$, but for $c > 1$ we must use a recursion relation [6] defined by solving Eq. (2) for $\bar{\rho}_{j+1}$ in terms of the other densities. For $c > 1$ we can use multiple upwind steps in order to derive the low-order solution (see Steinle and Morrow [6]).

Once the high- and low-order solutions are known, the antidiffusive fluxes can be determined by computing in the direction of the flow, away from the upstream boundary, the anti-diffusive flux

$$\phi_{j+1/2} = \tilde{\rho}_j - \bar{\rho}_j + \phi_{j-1/2}. \tag{7}$$

This is the most rapid method of computing the antidiffusive fluxes, for all c.

Once the anti-diffusive have been obtained they must be limited to prevent the development of unwanted maxima and minima using either Boris and Book's limiter [5] or Zalesak's limiter [7]. We find little difference between the two methods. Here we use the more efficient Boris and Book limiter to produce the corrected fluxes, $\bar{\phi}_{j+1/2}$, which are then applied to give the final solution

$$\rho_j^{n+1} = \tilde{\rho}_j - \bar{\phi}_{j+1/2} + \bar{\phi}_{j-1/2}, \tag{8}$$

where ρ_j^{n+1} is the final solution at time $t + \delta t$ and mesh point j.

The remaining problem is that we have one method of solution for $c > 1$ and a different method for $c \leqslant 1$, and we must match the two methods of solution about the transition point where $c = 1$. Note that we need only consider the case where $c > 0$, as the case where $c \leqslant 0$ can be derived by symmetry.

When a transition is required in a region of decreasing c the solution may be marched to the transition point, then the transition point is used as a boundary condition for the tridiagonal system of equations used for $c \leqslant 1$. For the alternate case we use the upwind solution to close the system of equations. It is generally found that the overall accuracy of a scheme is not affected by using the low-order method at one point.

Using the above method the transition from one method of solution to the other can be achieved without any distortion.

3. Results and Discussion

3.1. *Analytic Solution in a Linear Velocity Field*

If we assume a linear variation of velocity with position of the form

$$w = k(d - x), \tag{9}$$

where k and d are constants, then by considering the solution of Eq. (1) along characteristics, one can show that an initial distribution of the form

$$\rho(x, 0) = \rho_0(x) \tag{10}$$

becomes

$$\rho(x, t) = \rho_0((x-d)\, e^{kt} + d)\, e^{kt}. \tag{11}$$

We can thus predict the change in the shape of any initial waveform with time in a linearly varying velocity field and we use this as a basis for testing the accuracy of numerical solution for both square and semi-circular waveforms.

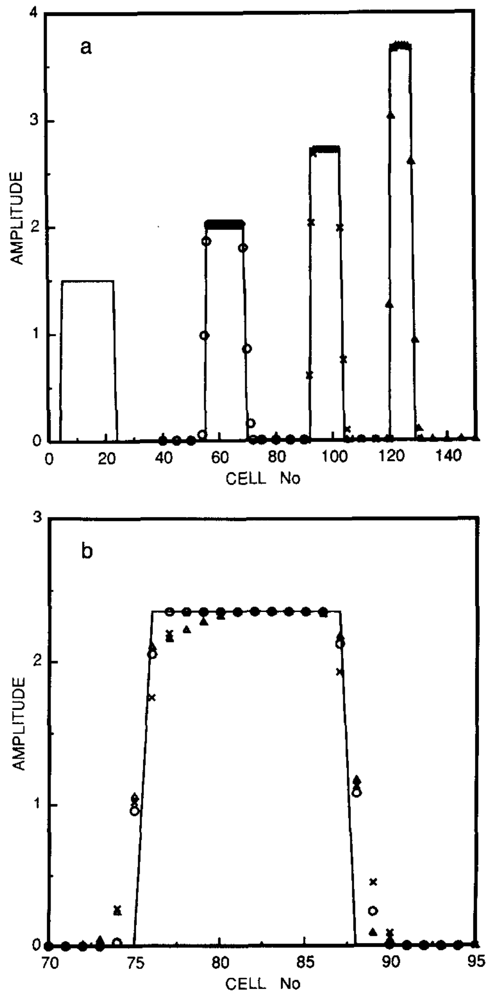

FIG. 1. The square-wave test with a decreasing velocity field: (a) The fourth-order method with c varying from $c=1$ at cell 0 to $c=0$ at cell 200. The computed results after 61 time steps, ○, 121 time steps, ×, and 181 times steps, △, are compared with the exact solution ———. The initial square-wave of amplitude 1.5 from cell 4 to 24 is also shown. (b) Detailed comparison with the exact solution; ———, of results obtained using (i) the fourth-order method, 91 steps with $0 \leqslant c \leqslant 1$, ○, (ii) the SHASTA method, 181 steps with $0 \leqslant c \leqslant 0.5$, ×, (iii) the marching method, 23 steps with $0 \leqslant c \leqslant 4$, △.

3.2. *Numerical Results*

We compare the solutions obtained with the Phoenical LPE SHASTA algorithm and the fourth-order algorithm with the exact solution for the square-wave test [6] in Fig. 1 and for the semi-circle test [6] in Fig. 2. In all cases shown the velocity decreases linearly from a value at cell 0 which determines the maximum value of c, c_{max}, to zero at cell 200. For the SHASTA method $c_{max} = 0.5$, for the fourth-order method $c_{max} = 1$ to demonstrate the tri-diagonal matrix inversion method of solution, and then $c_{max} = 4$ to demonstrate the performance of the recursion method of solution for $c > 1$. Figures 1a and 2a show the movement and distortion of the

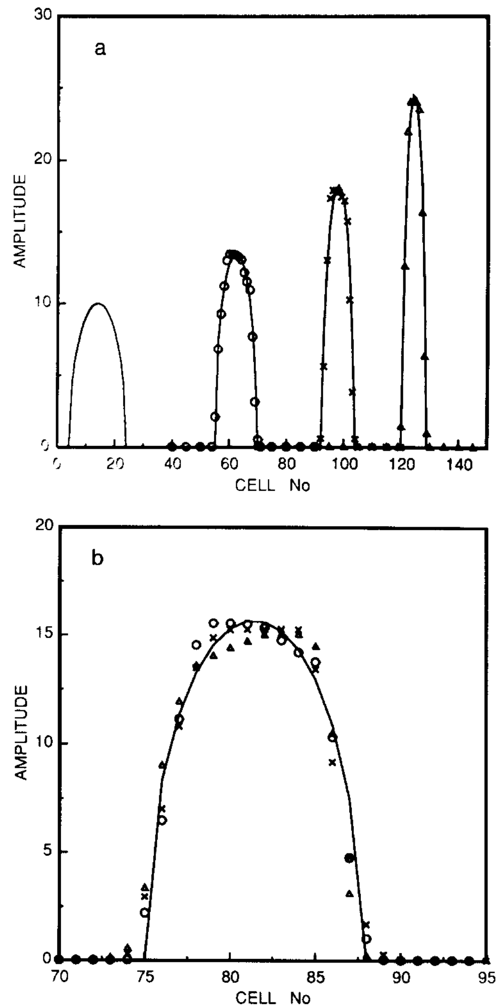

FIG. 2. The semi-circle test with a decreasing velocity field: (a) The fourth-order method with conditions and symbols as for Fig. 1a. (b) Detailed comparison with the exact solution with conditions and symbols as for Fig. 1b.

TABLE I

The Average Error (A.E.) Values and Computational Times for the Square-Wave and Semi-Circular Wave Tests in a Decreasing Velocity Field

Method	Range of c	No. of steps	A.E. (square-wave)	A.E. (semi-circle)	CPU time (s)
LPE SHASTA	0.5...0	181	0.0596	0.2053	30
4th order	0.5...0	181	0.0454	0.1941	44
	1...0	91	0.0410	0.1888	22
	2...0	46	0.0403	0.2382	11
	3...0	31	0.0509	0.2310	8
	4...0	23	0.0708	0.2383	7

waveforms with time. Figures 1b and 2b compare in detail the solutions after the same time has elapsed, which is after 181 time steps for the SHASTA method, 91 time steps for the fourth-order method with $c \leqslant 1$, and only 23 time steps for the fourth-order method using the recursion relation [6] for $c \geqslant 1$. In Table I the computational times and the average error (A.E.) are given for each test. The average error is computed from the formula A.E. $= \frac{1}{100} \sum_j |\rho_j^* - \rho_j^n|$, where the range of j covers all regions where the computed ρ_j^n and the exact solution ρ_j^* differ. Note that A.E. values are only relative, and the square-wave results must not be compared with the semi-circle results.

From the square-wave propagation results shown in Fig. 1b it is clear that the implicit solution for $c \leqslant 1$ is less diffused than the SHASTA solution with the density change more sharply defined, as reflected in the A.E. values of Table I, and takes less computational time, also shown in Table I. For $c > 1$ the fourth-order method is less accurate than the SHASTA method, but gives quite acceptable results with all the monotonic non-oscillatory properties of an F.C.T. method, in less than a quarter of the time and in one eighth the number of time steps. Similar comments apply to semi-circle tests; however, it should be noted that the clipping action of the flux-limiter has a modifying effect on the results for this test, particularly as the profiles become very sharp.

TABLE II

The average Error (A.E.) Values and Computational Times for the Semi-Circular Wave Tests in an Increasing Velocity Field

Method	Range of c	No. of steps	A.E. (semi-circle)	CPU time (s)
LPE SHASTA	0...0.5	81	0.1145	14
4th order	0...0.5	81	0.1091	20
	0...1	41	0.1094	10
	0...2	21	0.1300	5
	0...4	11	0.1566	3

Tests were also made with linearly increasing velocity fields and the results of these tests are summarised in Table II. The level of error is less since the wave profiles expand in this case. The relative accuracy of each method is similar to that described above for the decreasing velocity field.

4. Summary

We have developed an analytic method of describing the distortion of an arbitrary waveform advecting in the presence of a linearly varying non-uniform velocity field. This development is important since transport algorithms have been used in highly non-uniform velocity conditions in numerous gas-discharge applications without any analytic tests of their behaviour under these conditions.

The analytic method has been applied in the case of square- and semi-circular waveforms to test the accuracy of the Phoenical LPE SHASTA algorithm and the newly developed implicit fourth-order FCT algorithm. Velocity distributions both linearly increasing and linearly decreasing with distance are tested and the results are generally very good. The fourth-order implicit method is generally more accurate than the SHASTA method, and for $c > 1$ comparable accuracy can be obtained with a threefold decrease in the computational time required over the SHASTA method. Of even greater importance in some cases is the reduction in the total number of time steps required for a given order of accuracy. For example, in gas discharge calculations the solution of Poisson's equation at each time step takes more time than the solution of the transport equations.

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