Noreddine BENAIRED, Ali HENNAD

University of Sciences and Technology of Oran Mohamed Boudiaf , USTO-MB, FGE-LMSE, BP 1505 El M'Naouer, 31000 Oran, Algeria

ADBQUICKEST Numerical Scheme for Solving Multi-Dimensional Drift-Diffusion Equations

Abstract *– We present in this work a multi-dimensional resolution of the Drift-Diffusion equations using the numerical scheme ADBQUICKEST coupling at time splitting method. This will allow us to study the dynamics of particles in the case of electrical discharge to understand their propagation. The obtained results are compared to analytic solutions and to those found in the literature.*

Streszczenie. *W artykule zaprezentowano wielowymiarowe rozwiązanie równań Drift-Diffusion z wykorzystaniem metody ADBQUICKEST. Zaproponowane rozwiązanie pozwala na analizę dynamiki cząstek w stanie wyładowania elektrycznego.* ***Rozwiązanie wielowymiarowe równań Drift-Diffusion z wykorzystaniem metody ADBQUICKEST****.*

Keywords: ADBQUICKEST Scheme, Drift-Diffusion, 3D Modeling, Time Splitting Method
Słowa kluczowe: metoda ADBQUICKEST, równania Drift-Diffusion, wyładowanie elektryczne

doi:10.12915/pe.2014.08.20

Introduction

Numerical simulation of the transported particles dynamics in an electrical discharge is based on the choice of algorithms to solving the numerical model equations of this discharge. For example the modeling of filamentary gas discharges like streamers.

Many researchers are interested in numerical modeling to solve the Drift-Diffusion equations. A numerical multi-dimensional modeling requires the use of a powerful numerical scheme that can, on the one hand, following the strong density gradients and other it is desirable that this scheme is flexible and consumes little computing time for a simple and easy operation. So the algorithms used must meet the constraints of the physical phenomenon and the requirements of computation time. Our work is devoted to the development of an efficient multi-dimensional numerical model to solve the transport equations [1].

Numerical Model

The one-dimensional equation of Drift-Diffusion is defined by:

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

With:

$$\Phi(x,t)=n(x,t)W-D\frac{\partial}{\partial x}n(x,t) \tag{2}$$

The Quickest scheme (Quadratic Upstream Interpolation for Convective Kinematics with Estimated Streaming Terms) was described and developed by Leonard [3]. It does not require special knowledge of the solution, and can address all points of interval between the electrodes in the calculation.

The use of flow in the Quickest scheme can generate the appearance of new maximum density and thus reintroduce negative densities. This is the role of the feed limiter as ADBQUICKEST technique which is the latest among the techniques described in the literature [4][5] [6].

The ADBQUICKEST method is a new version of the TVD (Total Variation Decrease) Quickest scheme. It was presented for the first time in the literature in 2009 by Ferreira and Kurokawa [5]. They have discretized the continuity equation using the finite difference method in the third order. Writing the continuity equation using this type of discretization is called the Quickest algorithm.

Coupling the Quickest scheme with the flow limiter ADBQUICKEST present a better alternative for solving multi-dimensional problems of Drift-Diffusion equations. This technique is based on the calculation of the flow by the equation:

$$\Phi^k_{i+1/2}=\frac{1}{2}\left[(n^k_{i+1}+n^k_i)-c(n^k_{i+1}-n^k_i)\right]-\frac{(1-c^2)}{6}(n^k_{i+1}-2n^k_i+n^k_{i-1}) \tag{3}$$

c: is the number of current (criterion of Friedrich-Levy: CFL) given by the expression:

$$c=c_{i+1/2}=W_{i+1/2}\ \frac{\Delta t}{\Delta x} \tag{4}$$

The use of flow $\Phi^k_{i+1/2}$ in the numerical scheme can introduce fictive densities and make appear a new maximum density. This is the role of the flow limiter that must realize respecting the non-creation of new extrema or sharpening existing extremes.

The ADBQUICKEST scheme flow limiter is given by the expression [5][7]:

$$\Phi(r^k_{i+1/2})=max\left[0,min\left[2\ r^k_{i+1/2},G,2\right]\right] \tag{5}$$

With:

$$G=\frac{1}{3(1-|c|)}\left[2+c^2-3|c|+(1-c^2)\ r^k_{i+1/2}\right] \tag{6}$$

and

$$r^k_{i+1/2}=\frac{n^k_i-n^k_{i-1}}{n^k_{i+1}-n^k_i} \tag{7}$$

The majority of algorithms for solving the continuity equation give the calculated solution in the following form:

The ADBQUICKEST technique can be developed, also, as follows:

The equation (1) can be written after discretization and by the use of the method of finite differences as:

$$n^{k+1}_i-n^k_i=-(\frac{A}{\Delta t}c_{i+1/2}-\frac{B}{\Delta t}c_{i-1/2}) \tag{8}$$

With:

$$\text{A}=\int_0^{\Delta t}n(x_{i+1/2},t)\ dt \quad \text{and} \quad \text{B}=\int_0^{\Delta t}n(x_{i-1/2},t)\ dt \tag{9}$$

if we consider that the velocity is constant within each interval, the equations (8) and (9) are expressed only in terms of the density $n(x,t)$ and the number of current $c=c_{i+1/2}$, it follows that:

$$n^{k+1}_i-n^k_i=-c\ (n^k_{i+1/2}-n^k_{i-1/2}) \tag{10}$$

With:

$$n^k_{i\pm 1/2}=\frac{1}{\Delta t}\int_0^{\Delta t}n\ (x_{i\pm 1/2},t)dt \tag{11}$$

$n_{i+1/2}^{k}$ and $n_{i-1/2}^{k}$ represent the mean value taken over the time interval Δt of the densities at the center of each cell.

The primary ADBQUICKEST technical objective is to control the values $n_{i+1/2}^{k}$ and $n_{i-1/2}^{k}$ from the schema Quickest to make strictly positive pattern and so that no maximum or minimum appears in the time interval.

In what follows, we perform numerical tests on the algorithm used in this work. These tests will allow us to choose the algorithm that more accurately meets the above criteria.

This numerical experience will be carried out by spreading the density profile with a constant velocity over one period T given by:

(12) $$T=\int_0^1 \frac{1}{W(x)}dx .$$

The constant propagation velocity $W(x)$ is equal to 10 ($a.u.$).

The resolution of the continuity equation (without diffusion term and with no source term) is made for the points number n_x equal 100 at 500 along the propagation axis.

The numerical scheme must be able to follow as closely as possible the analytical distribution of the initial multi-form density $n(x,t)$: rectangular, Gaussian, triangular, with a constant drift velocity.

This density is given at the initial time by the following expression:

$n(x)=10$ for $0.05\le x\le 0.25\ \ (a.u.)$

$n(x)=10\,exp\left[-300(x-0.5)^2\right]$ for $0.35\le x\le 0.65\ \ (a.u.)$

$n(x)=100x-75$ for $0.75\le x\le 0.85\ \ (a.u.)$

$n(x)=-100x+95$ for $0.85\le x\le 0.95\ \ (a.u.)$

$n(x)=0$ in the rest of the interval

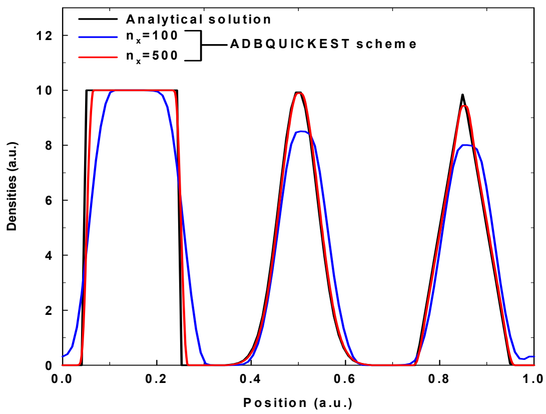

Fig. 1: Calculated solutions at the instant $t= T$.

Figure (1) shows the calculated results at the instant T for a constant propagation velocity. The number n_x is equal to 100 and 500 and the interval between the electrodes is equal to 1 ($a.u.$).

We note that the profile of the calculated solution using the ADBQUICKEST numerical scheme is consistent with the analytical solution profile (for n_x=500).

Application of the numerical scheme for transport equations ADBQUICKEST

a. Mono-dimensional resolution

Because of its qualities of stability, precision and fastness, we can say that the use of ADBQUICKEST method has opened new perspectives for modeling non-equilibrium electrical discharges.

It is proposed to solve the Drift-Diffusion equations in Cartesian geometry. We choose to illustrate the formalism, the plane-plane configuration.

To validate our numerical scheme using the ADBQUICKEST algorithm, we study the density profile solution in the case of test situations where the solution is already known. It is the propagation of a rectangular initial density profile with drift velocity $W(x)$. This velocity is independent of time and may vary according to the position according to the following expression:

(13) $$W(x)=1+9\sin^9(\pi x)$$

It has a maximum for the position of x=0.5 which is ten times larger than its value at the beginning and the end of the interval (at x=0 and x=1 positions).

The initial density distribution $n(x,t)$ is such that:

$n(x)=10$ for $0.05\le x\le 0.25\ \ (a.u.)$

$n(x)=0$ in the rest of the interval

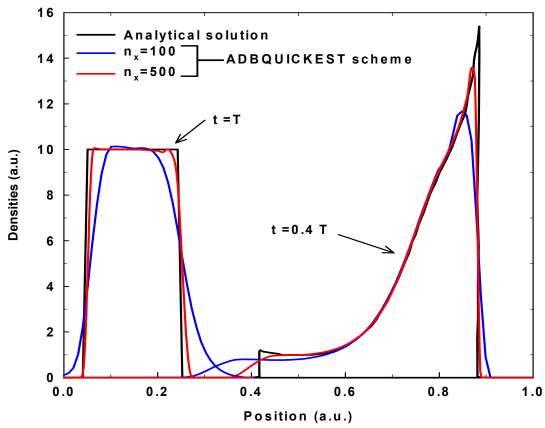

Fig. 2: Calculated solutions at the instants $t=0.4T$ and $t= T$.

Figure (2) represents the analytical solution and the calculated solution according to the position by using the ADBQUICKEST scheme at the instants $t=0.4T$ and $t=T$, for the points number n_x equal 100 at 500.

We note that the profiles of the calculated solution (for n_x=500) at $t=0.4T$ and $t=T$ are substantially similar to the profiles of the analytic solution to these instants.

The peak profile obtained from the analytical solution by Davies [8] at $t=0.4T$ has been almost achieved. At the instant t=T, we are seeing a slight distortion in the corners of the rectangular form.

This behavior is due to the discontinuity at the edges of the profile used and the correction made by the ADBQUICKEST scheme that ensures the removal of any extremum.

The calculation of the Mean Absolute Error (MAE), tells us about the accuracy and quality of the used method. The absolute error is calculated after one period T depending on the value of the position and using many values of the CFL (10^{-3} to 0.8).

The choice of these values of the CFL is justified by the different research done in the literature [9][10][11]. This error is given by the following equation:

(14) $$MAE=\frac{1}{n_x}\sum_{i=1}^{nx}\left| n_i^T - n_i^{analytic}\right|$$

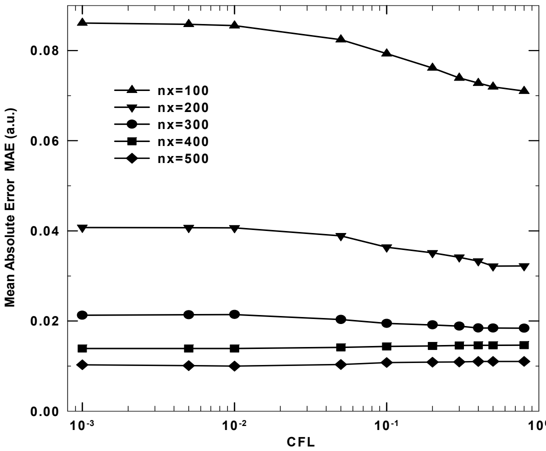

Fig. 3: ADBQUICKEST Mean Absolute Errors.

Figure (3) shows the variation in the mean absolute error as the function for several values of n_x points number (100 to 500 points) and CFL (10^{-3} to 0.8). We can notice that the value of the mean absolute error is almost independent of the CFL (n_x eq. 100 to 500) and inversely proportional to the n_x number. We conclude that the ADBQUICKEST is a conservative scheme.

b. Two-dimensional resolution

The extension of the previous one-dimensional resolution to two dimensions in cylindrical coordinates can be considered using the Time Splitting method.
This method is to consider the two-dimensional numerical problem described by the following equation:

$$\frac{\partial n}{\partial t}+\frac{\partial \Phi_z}{\partial z}+\frac{1}{r}\frac{\partial (r\,\Phi_r)}{\partial r}=0 \tag{15}$$

$$\Phi_z = nW_z - D_z\frac{\partial n}{\partial z} \tag{16}$$

$$\Phi_r = nW_r - D_r\frac{\partial n}{\partial r} \tag{17}$$

The equation (15) can be reduced to series problems in one dimension [12] [13] [14].
This means that the transport of the particles which occurs synchronously linked in the space and time will be carried separately by solving first the transport equation in the axial direction:

$$\frac{\partial n}{\partial t}+\frac{\partial \Phi_z}{\partial z}=0 \tag{18}$$

The calculated density is introduced to solve this equation in the radial direction:

$$\frac{\partial n}{\partial t}+\frac{1}{r}\frac{\partial (r\,\Phi_r)}{\partial r}=0 \tag{19}$$

With: W_z and W_r the axial and radial drift velocities. The diffusions coefficients (D_z and D_r) are considered zero.

To validate our numerical scheme in 2D, we will use the calculation parameters proposed by Flitti [15].
This is to follow the spatiotemporal evolution of a known form initial density. The axial and radial points number equal to 100 (r and z $\in\left[0,10^{-2}\right]$ $(a.u.)$). The diffusion coefficient and the source term are zero. The axial and radial drift velocities are the same as those used by Flitti [15].

The initial density used in this test is a Gaussian profile given by the following expression:

$$n(z,r)=n_1\, e^{\frac{-(z-z_0)^2-(r-r_0)^2}{\sigma^2}} \quad (a.u.) \tag{20}$$

For which; the values of n_1, z_0, r_0 and $\sigma 2$ are given respectively as follows: 10^{12}, 0.9, 0.9 and 0.04 in arbitrary units.

Figure 4 shows the 2D Gaussian profile of the initial density presented in arbitrary units.

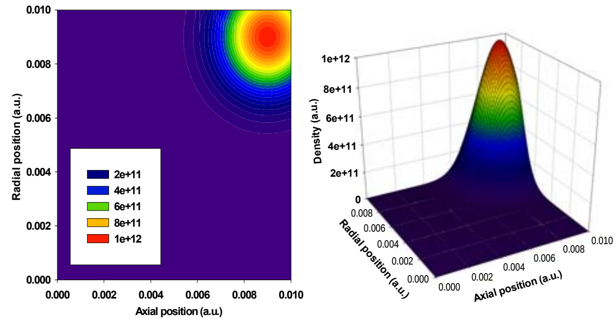

Fig.4: Initial density in arbitrary units.

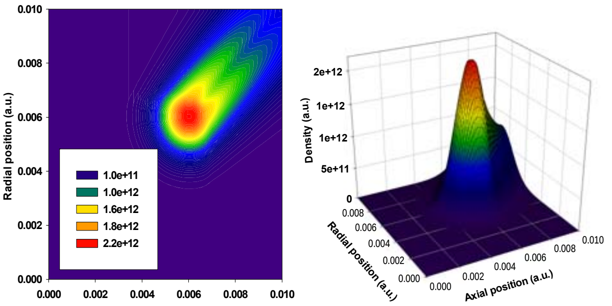

Fig. 5: Density propagation in diagonal direction $(a.u.)$.

The diagonal propagation of the density is due to axial and radial drift velocities of equal values. This profile of the density, as shown in Figure (5) is consistent with that found by the Scharfetter and Gummel scheme used in Benaired thesis [9].

c. Three-dimensional resolution

The three-dimensional resolution of the Drift-Diffusion equation for particles density can be done by adopting the above method called Time Splitting:
In the longitudinal direction:

$$\frac{n^{k+1}_{i,j,l}-n^{k}_{i,j,l}}{\Delta t}+\frac{\Phi^{k}_{i+1/2,j,l}-\Phi^{k}_{i-1/2,j,l}}{\Delta x}=0 \tag{21}$$

In the transversal direction:

$$\frac{n^{k+1}_{i,j,l}-n^{k}_{i,j,l}}{\Delta t}+\frac{\Phi^{k}_{i,j+1/2,l}-\Phi^{k}_{i,j-1/2,l}}{\Delta y}=0 \tag{22}$$

According to the tangential direction:

$$\frac{n^{k+1}_{i,j,l}-n^{k}_{i,j,l}}{\Delta t}+\frac{\Phi^{k}_{i,j,l+1/2}-\Phi^{k}_{i,j,l-1/2}}{\Delta z}=0 \tag{23}$$

Then, the source term is introduced:

$$\frac{n^{k+1}_{i,j,l}-n^{k}_{i,j,l}}{\Delta t}=S^{k}_{i,j,l} \tag{24}$$

In order to validate the numerical scheme in 3D, we used this time an initial density of spherical form that is shown in Figure (6) with constant velocity propagation equal to 10 $(a.u.)$ in the longitudinal direction.

The points number in the longitudinal direction is n_x=120 ($x\in\left[0,0.5\right]$ $(a.u.)$). In the transversal and tangential directions n_y=n_z=60 ((y and z $\in\left[-0.2,0.2\right]$ $(a.u.)$). The initial density used in this test is given by the following expression:

$$n(x,y,z) = n_1\, e^{\frac{-(x-0.1)^2-y^2-z^2}{\sigma^2}} \quad (a.u.)$$

For which; the values of n_1 and σ are given respectively as follows: 10^{14} and 0.027 in arbitrary units.

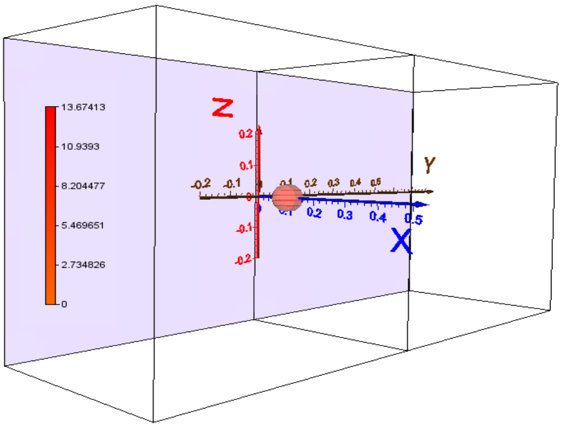

Fig. 6. 3D representation at t=0 of initial density $\log_{10}(n(x,y,z,t))$.

Figure (7) shows the density propagation at the time t = 0.4T along the axis without deformation in the initial density profile, confirming that the ADBQUICKEST is a conservative scheme.

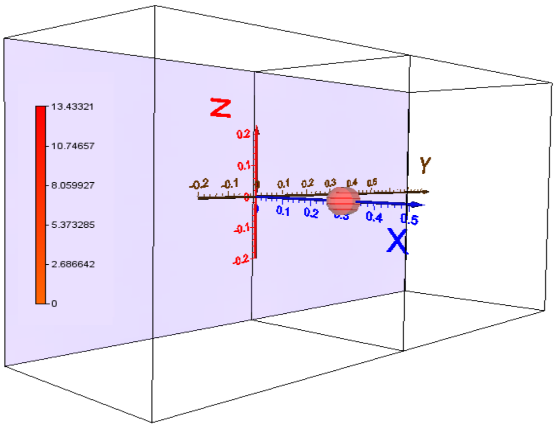

Fig. 7. 3D representation at $t=0.4T$ of density $\log_{10}(n(x,y,z,t))$.

The presentation of the results in three dimensions allows us to see the volume distribution of the calculated density. This presentation is very different from the classical presentation includes only 2D surfaces in three dimensional space.

Conclusion

The objective of this study was to develop an efficient numerical model based on the ADBQUICKEST scheme for solving Drift-Diffusion equations in multi-dimensional geometry. To validate our numerical scheme using the ADBQUICKEST algorithm in multi-dimensions, we have compared the obtained results to the analytic solutions founded in the literature. This validate model allow us, in the future, to study the dynamics of charged particles in the case of high pressure electrical discharge to a better understanding of the evolution and propagation of ionization waves in situations of high density variations and electric field.

Nomenclature

n	Number density
Φ	Species flux
W	Drift velocity
D	Diffusion coefficient of species
c	Current number criterion of Friedrich-Levy
Δt	Temporal step
Δx	Longitudinal spatial step
Δy	Transversal spatial step
Δz	Tangential spatial step
Δr	Radial spatial step

REFERENCES

1 Chao Li, Ebert U and Hundsdorfer W.Spatially hybrid computations for streamer discharges. Journal of Computational Physics Volume 231 Issue 3, (2012)
2 Dhali P. F, Williams, Two dimensional studies of streamers in gases J. Appl. Phys. Volume 62 / Issue 12 (1987), 4696.
3 Leonard. B. P. The QUICK algorithm: a uniformly third-order finite difference method for highly convective flows. Computer Methods in Applied Mechanics and Engineering, (1979), 19, 59
4 Caro Candezano M., Sartori P., Simões A., Ferreira V.G.. Numerical solutions of shallow water equations with source term using high resolution bounded upwind schemes. 10a Conferencia Brasileira de Controle e Aplicaçoes (2011)
5 Ferreira V.G., Kurokawa F.A., Queiroz R.A.B., Kaibara M.K., Oishi C.M., Cuminato J.A., Castelo A., Tomé M.F., McKee S. Assessment of a high-order finite difference upwind scheme for the simulation of convection-diffusion problems. International Journal of Numerical Methods in Fluids, Vol. 60, No. 1-26 (2009).
6 Miguel A. Caro Candezano,. Valdemir G. Ferreira. A comparative study of upwind differencing schemes in the context of schock capturing properties. CNMAC, (2010) ISSN 1984-820X. Publication SBMAC V.3
7 Waterson NP, Deconinck H. Design principles for bounded higher-order convection schemes—a unified approach. Journal of Computational Physics 2007; 224:182–207.
8 Davies A.J., Niessen W. The Solution of the Continuity Equations in Ionization and Plasma Growthy. And Appl. Of Pseudosparks, Gundersen Schafer New York, 1990.
9 Benaired N.. Modélisation hydrodynamique en 3D d'une décharge filamentaire à haute pression. Doctoral thesis. USTO-MB University. 2013
10 Ferreira V. G, Kaibara M. K, Lima G. A. B, Silva J. M., M. Sabatini H, Mancera P. F. A, McKee S. A robust TVD/NV-based upwinding scheme for solving complex fluid flow problems. October 2010
11 Lima G. A. B, Ferreira V. G, Queiroz R. A. B, Miguel A. Caro Candezano, Development and evaluation of two new Upwind schemes for conservation laws. 20th International Congress of Mechanical Engineering. November 15-20, 2009, Gramado, RS, Brazil
12 Bessieres D. Modélisation des décharges filamentaires. Thèse de Doctorat. Université de Pau et des pays de l'Aldour. 2006
13 Hundsdorfer W., Portero L. A Note on Iterated Splitting Schemes Journal of Computational and Applied Mathematics 201(2007)146–152.
14 Benaired N. and Hennad A. Three-dimensional modelling of filamentary discharge using the SG Scheme coupling at time splitting method, Przeglad Eektrotechniczny, ISSN 0033-2097, R. 89. NR: 1a/2013.
15 Flitti A. Modélisation numérique 1.5D et 2D de la propagation d'une décharge filamentaire haute pression. Doctoral thesis. USTO MB Oran. November 2007.

.

Authors

Noreddine Benaired *(Dr) is doctor at University center of Relizane, Algeria. E-mail: nbenaired@yahoo.fr*

Ali Hennad *(Pr) is currently a Professor at University of Sciences and Technology of Oran, Algeria.*
E-mail: ali_hennad@yahoo.fr