ELSEVIER

Nuclear Instruments and Methods in Physics Research A 421 (1999) 234–240

NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH Section A

Monte Carlo simulation of electron drift and diffusion in counting gases under the influence of electric and magnetic fields

S.F. Biagi

Department of Physics, Oliver Lodge Laboratory, The University of Liverpool, Liverpool L69 7ZE, UK

Received 20 July 1998; received in revised form 26 August 1998

Abstract

A fast and accurate computer simulation program for electron drift and diffusion in gases under the influence of electric and magnetic fields is described and some calculated results are compared to precise experimental results in carbon tetraflouride and methane mixtures. The calculated Lorentz angles are shown to be typically within 1° of the measured experimental values. The program allows the electric and magnetic fields to be at any angle to each other.

1. Introduction

The modeling of electron motion in gas avalanche radiation detectors can help in the optimisation of their design in many different detector geometries. The combination of the gas simulation program Magboltz [1] and electric field simulation programs Garfield [2] or Maxwell [3] has been used in many current and future detector designs for experiments in high energy and nuclear physics.

The present work was stimulated by the observed break down in the accuracy of the predictions of Magboltz in some gases at large magnetic fields. This loss of accuracy was caused by some of the approximations used in the Magboltz program and occurs in simulations in large magnetic fields with a gas having a cross-section with a deep Ramsauer minimum. The Boltzmann transport equation solved in Magboltz uses a solution for the energy distribution function which is an expansion in Legendre polynomials. The standard solution of the Boltzmann transport equation truncates the energy distribution expansion after the first two terms of the Legendre polynomials, the Magboltz program uses an expansion up to the third Legendre polynomial which was found useful in improving the computational accuracy of the drift velocity to better than 1%. Higher terms in the expansion would improve the accuracy further but require a large increase in computation time.

Recently, Ness [4,5] has extended the multi-term formalism to the case of transverse electric and magnetic fields using the more general expansion of the distribution function in spherical harmonics. The results from Ness [5] served as a benchmark test for the accuracy of the Lorentz angle calculations using the Maxwell model and the Reid Ramp and Step models [6]. The calculations using the Magboltz program gave good agreement with the Maxwell model, but deviations of up to 10% in the Lorentz angles were observed with the results from the Ramp and Step models [5]. The reasons

0168-9002/99/$ – see front matter
PII: S0168-9002(98)01233-9

for this behaviour are well known and stem from the large anisotropy in the velocity of the electrons in the direction of the electric field. This anisotropy is poorly simulated if the truncation of the energy distribution function is not taken to a large number of terms in the spherical harmonics or Legendre polynomials.

In order to improve the simulation and also guarantee the calculation accuracy to better than 1% for the Lorentz angle the Monte Carlo integration technique was applied to the solution of the transport equations. This technique is independent of the expansions used in describing the electron energy distribution and gives guaranteed convergence to an accuracy which is dependent only on computation time.

2. The Monte Carlo integrator

The Monte Carlo integration technique in the case of an electric field has been previously described by Fraser and Mathieson [7]. We only discuss here the differences due to the extension of their algorithms to include the magnetic field at any angle to the electric field. The collision types involved have been extended from elastic and inelastic collisions [7] in order to include also, attachment, ionising and super-elastic collisions. The collision angular distributions have also been introduced using a new technique [9].

The inclusion of a magnetic field introduces some complications in the movement of the electron. In order for the calculation to be executed as quickly as possible it is necessary to introduce an analytic description of the electron motion rather than to integrate along the electron path.

If the magnetic field, B, is taken along the X-axis and the electric field, E, is at an angle, Φ in the $X-Z$ plane the equations of motion can be given analytically. The electric field is now decomposed into components:

$$E_X = E\cos\Phi \quad \text{and} \quad E_Z = E\sin\Phi.$$

The cyclotron frequency is given by $W = eB/m$ where e and m are the charge and mass of the electron. The turning angle, Ω, in the magnetic field in a time, ∂t, between collisions is:

$$\Omega = W\partial t.$$

Given an initial spatial position X_0, Y_0, Z_0 and a velocity V_{X0}, V_{Y0}, V_{Z0} the updated position X_1, Y_1, Z_1 and velocity V_{X1}, V_{Y1}, V_{Z1} of the electron after a time, ∂t, is given by

$$X_1 = X_0 + V_{X0}\,\partial t + 0.5e/mE_X\partial t^2,$$

$$Y_1 = Y_0 + 1/W[(V_{Y0} - E_Z/W)\sin(\Omega) + V_{Z0}(1-\cos(\Omega)) + E_Z\partial t],$$

$$Z_1 = Z_0 + 1/W[V_{Z0}\sin(\Omega) - (V_{Y0} - E_Z/W)(1-\cos(\Omega))],$$

$$V_{X1} = V_{X0} + e/mE_X\partial t,$$

$$V_{Y1} = (V_{Y0} - E_Z/W)\cos(\Omega) + V_{Z0}\sin(\Omega) + E_Z/W,$$

$$V_{Z1} = V_{Z0}\cos(\Omega) - (V_{Y0} - E_Z/W)\sin(\Omega).$$

The only unknown is the time step, ∂t, which is chosen by the null collision [8] technique. The position and velocity of the electron after the time ∂t can now be updated and so the motion of the electron through the gas is followed between collisions.

The angular distributions of elastic collisions are taken to be isotropic which implies that the cross-sections used are momentum transfer cross-sections. The momentum transfer formalism is exact if elastic collisions only occur, but in the case where elastic and inelastic collisions can occur this is no longer true. The inelastic collisions may have an anisotropic angular distribution and the inelastic scattering angular distribution needs to be included. The angular distribution for the elastic and inelastic levels are treated using the technique of Longo and Capitelli [9], this technique allows the angular distribution to be included by using both a momentum transfer inelastic cross-section, Q_{mn}, and the total inelastic cross-section, Q_{tn}, for excitation of a level n. The angular distribution is then given in terms of the forward scattering probability, P_n, where

$$P_n = 1/2 + (Q_{tn} - Q_{mn})/Q_{tn}.$$

The angular distribution algorithm now requires the selection of an extra random number to choose between forward and backward scattering. Once the choice of forward or backward scattering is made the next random number is used to give isotropic forward or isotropic backward scattering. Thus the minimum computation is maintained for the inclusion of angular distributions by using this relatively simple formalism. A further advantage is that phase shift analyses of electron scattering can give both the total and the momentum transfer cross-section in a self consistent manner from the same phase shifts.

The program outputs the drift velocity in the Cartesian coordinate system defined above as V_X, V_Y and V_Z. The general case where the magnetic field is not at right angles to the electric field leads to all three components taking finite values and has important consequences for the calculation of the diffusion tensor.

3. Calculation of the diffusion tensor

The diffusion can be calculated using either the displacement formalism or by using the correlation function between velocity and displacement, the Kubo [10] formalism. The Kubo formalism requires accurate knowledge of the drift velocity and is more computationally intensive when all three drift velocity components are finite. Therefore, the displacement formalism was used to give the diffusion tensor.

The diffusion is given as

$$D_{ij} = 1/(2N) \sum[1/\Delta t(X_i - V_i\Delta t)(X_j - V_j\Delta t)],$$

Where subscripts ij refer to the dimensions x, y or z. The spatial coordinates X_i, X_j and drift velocity components V_i, V_j of the electron are sampled at time intervals Δt separated by a number of collisions M. The summation is taken over the N collisions that are calculated in the N M total collisions of the simulation and M is chosen so that the error in the calculation of the diffusion coefficients is within a factor of two of the accuracy of the velocity vectors.

The diffusion is also calculated in the coordinate system aligned along the drift direction for the special case where the electric and magnetic fields are at right angles, then the diffusion is defined using only three components Dl, Dt and D_{xx} where Dl is the diffusion along the drift direction, Dt is the diffusion transverse to the drift direction and also transverse to the B field and D_{xx} is the diffusion transverse to the drift direction but parallel to the B field. This definition of the diffusion allows the easiest simulation of detector response in the common case where there are axial wires in a solenoidal B field.

The program outputs the calculated velocity and diffusion at an equally spaced number of collisions during the simulation, this allows the convergence of the calculation to be checked against the final calculated values. The time taken for convergence to better than 0.5% on the velocity and 1% on the diffusion is typically 10 s on a 200 MHZ DEC ALPHA computer for a typical counter gas mixture with 10 inelastic levels.

4. Results and discussion

The accuracy of the Monte Carlo program, Magboltz II, and Magboltz were checked with benchmark results [5] in model gases which serve as standard tests for simulation codes. These models, the Maxwell model and the Reid ramp and step models [6] and results obtained from them are discussed briefly below. The gases which requires the largest number of terms in the Boltzmann expansion to accurately describe their behaviour are carbon tetraflouride and methane; therefore, these gases and some of their counting mixtures were simulated with the Monte Carlo program and the results compared with recent accurate measurements in magnetic fields. The agreement of the measured Lorentz angles with predictions is shown to be typically within the experimental errors of 1° or 2° for very large Lorentz angles.

4.1. Model gases

4.1.1. Maxwell model

The Maxwell model is a model where the cross-section is inversely proportional to the square root of the electron energy. The collision frequency is

then constant independent of electron energy and the Boltzmann equation can be solved exactly. The results of Ness [5] have been tested with the Monte Carlo integrator and our results agree to within the statistical precision of our calculation (set to 0.1%) for both diffusion and drift velocity.The Maxwell model however is not a good test for the breakdown in the three term Legendre polynomial expansion that is used in Magboltz, identical results were obtained with Magboltz for this model. This reflects the fact that the electron energy distribution is highly isotropic in this model and only two or three terms in the Legendre polynomial expansion are required in order to obtain 0.1% accuracy.

4.1.2. Reid Ramp model

This model was originally introduced [6] to investigate the breakdown of the two term expansion of the energy distribution function in the Boltzmann equation. This model has properties which are much closer to real gases as used in radiation detectors and displays similar levels of breakdown in the two term expansion as seen in a 80/20 argon–methane mixture. The results of Ness [5] serve here as benchmarks against which the Monte Carlo integrator and the Magboltz program were checked for the case of perpendicular electric and magnetic fields. The results from the Monte Carlo integrator were again in excellent agreement, to 0.1%, with the results of Ness. The Magboltz program gave results for the Lorentz angle at some electric and magnetic fields which were in error by 10%, this inaccuracy was only observed with the magnetic field. When no magnetic field was used the velocity vector from Magboltz was always accurate to 1% demonstrating the increased sensitivity of the Boltzmann equation to higher terms in the expansion when a magnetic field is introduced.

4.2. Real gases

4.2.1. Carbon tetraflouride and methane

The requirements for fast detector response often lead to the use of carbon tetraflouride (CF_4), in radiation detectors. This gas obtains its high drift velocity because of the large Ramsauer dip in the elastic cross-section which coincides with a very large vibrational inelastic cross-section. Fig. 1 shows the CF_4 cross-sections; they consist of three vibrational levels, vibrational level harmonics at the 8 eV resonance and attachment, excitation and ionisation levels. Fig. 1 also shows the third vibrational level has a total and a momentum transfer cross-section, these are both required to describe the angular distribution of scattering from this level. The Monte Carlo program used here was ideally suited to the extraction of cross-sections for this gas because the accuracy of the simulation does not require the solution of the transport equations of a large number of terms in the expansion in Legendre polynomials or spherical harmonics. The cross-section set shown in Fig. 1 was derived starting from cross-sectional data of the electron scattering experiments [11–17], these were adjusted within the experimental errors to fit the data available from drift velocity, diffusion, attachment and ionisation measurements [18–24]. The experimental drift velocity and diffusion results, Figs. 2 and 3, display rather large disagreements at the 3 or 4% level between experiments and so unlike the case of methane, where experimental results agree at 1%, there is some uncertainty in the extracted cross-sections. This uncertainty is largest at energies below 0.12 eV. The experimental maximum

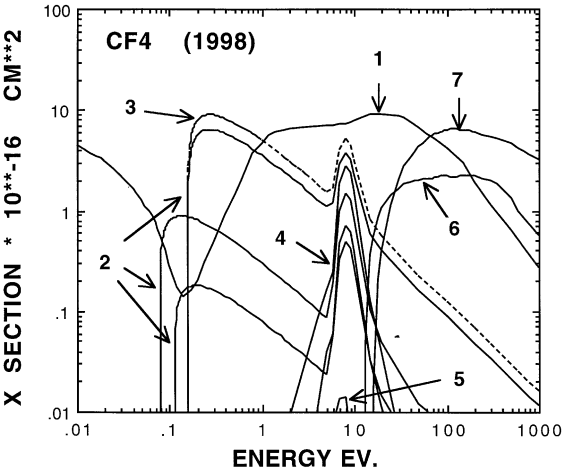

Fig. 1. Carbon tetraflouride cross-sections: (1) elastic, (2) vibrational (momentum transfer), (3) vibrational (total), (4) vibrational (harmonics), (5) attachment, (6) excitation and (7) ionisation cross-section.

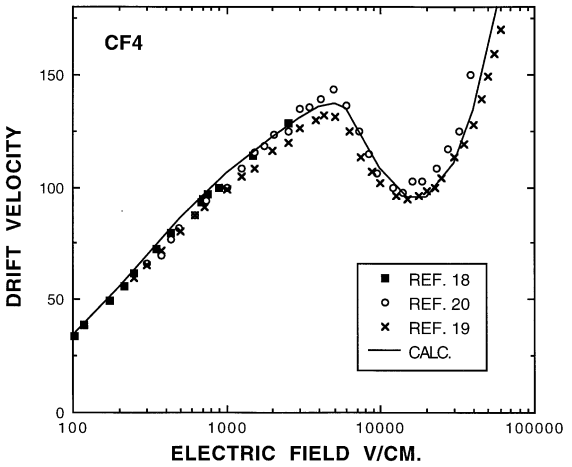

Fig. 2. Drift velocity in carbon tetraflouride.

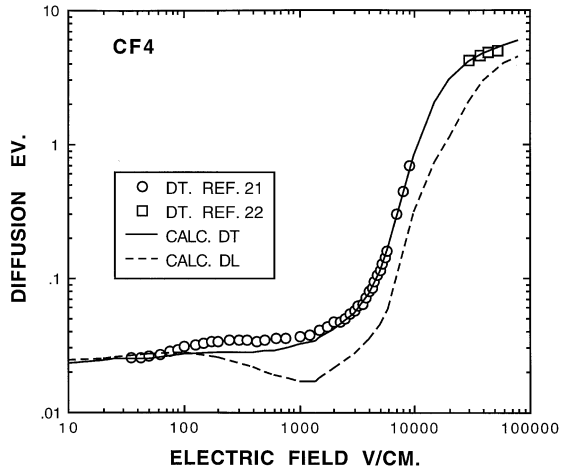

Fig. 3. Diffusion to mobility ratio in electron volts for transverse and longitudinal diffusion in CF_4.

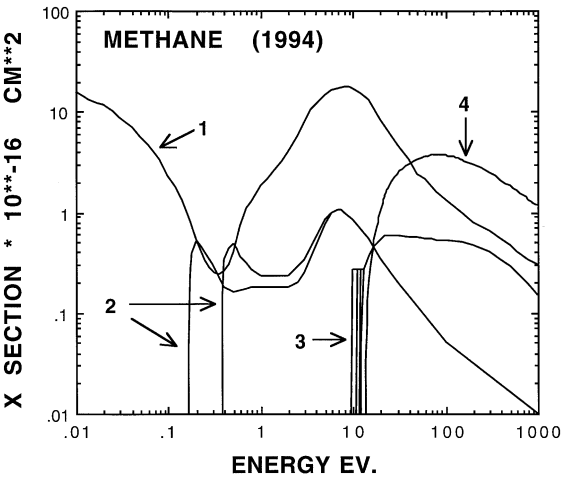

Fig. 4. Methane cross-sections: (1) elastic, (2) vibrational, (3) excitation (4 levels) and (4) ionisation cross section.

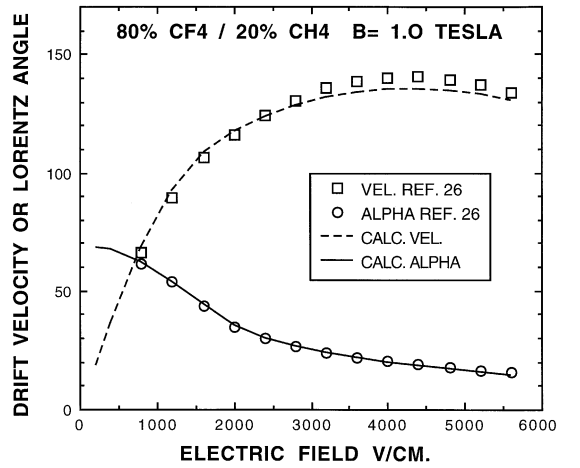

Fig. 5. Drift velocity and Lorentz angle in 80/20 CF_4/CH_4 at B = 1.0 T.

drift velocity is uncertain at the first drift velocity maximum and recent measurements vary between 133 and 140 micrometer/nanosecond, this uncertainty on the maximum drift velocity leads to some uncertainty on the angular distribution of the scattering from the third vibrational level. The ratio of the momentum transfer to total cross-section of the third vibrational level is particularly sensitive to the drift velocity maximum, this ratio was adjusted so that the calculated maximum drift velocity passed through the middle of the experimental drift velocity range. In all energy ranges the cross-sections agree well with electron scattering results.

Fig. 4 displays cross-sections for methane which are all isotropic since we obtained good fits to the published data without introducing angular distributions. These cross-sections are close to those previously used [1] but the vibrational inelastic scattering cross-sections have been increased by

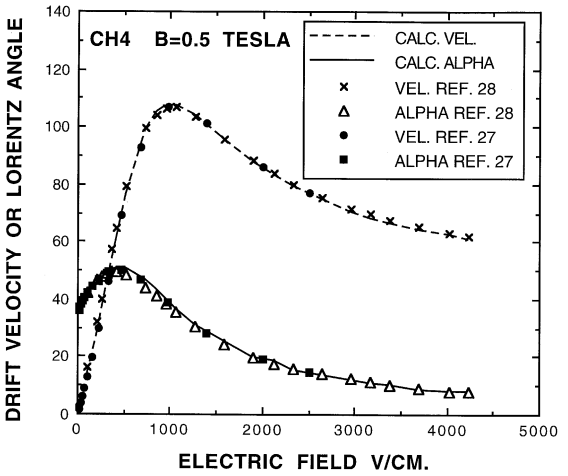

Fig. 6. Drift velocity and Lorentz angle in methane at $B = 0.5$ T.

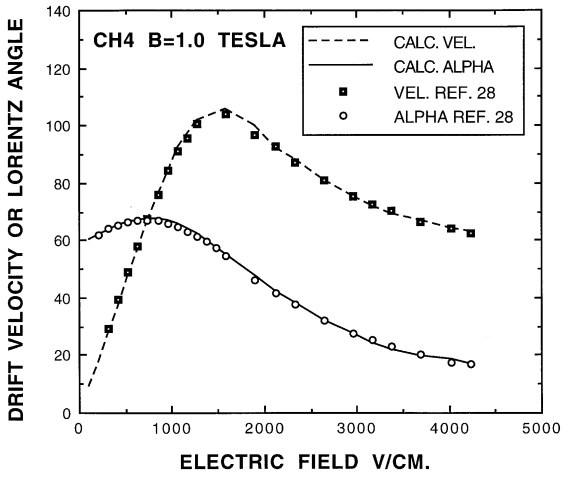

Fig. 7. Drift velocity and Lorentz angle in methane at $B = 1.0$ T.

5% to better fit new data [25] in mixtures of methane and noble gases.

Using these two cross-section sets we simulated the drift velocity and Lorentz angles in pure methane and a mixture of 80% CF_4 20% CH_4. The calculated results are shown in Figs. 5–7 and compared to measured data [26–28]. The agreement with measured Lorentz angles is typically within 1° for methane and methane–CF_4 mixtures. The total drift velocity is in very good agreement with the measured values at both 0.5 and 1.0 T in pure methane. The deviation of the prediction from experiment at the maximum drift velocity of the CH_4–CF_4 mixture can be traced to the fact that the experimental measurement at the maximum is from one of the sets of data that have high drift velocity and the cross-sections have been fit to the average data which contains both high and low values at the drift velocity maximum.

5. Conclusion

A simulation program has been written which is suitable for use in optimising the design of gas radiation detectors used in a magnetic field. It has been shown that approximately 1° accuracy can be obtained for the predicted Lorentz angle. The simulation is free from the complexities involved in solving the multi-term Boltzmann equation and is fast, taking about 10 s to produce a 0.5% accuracy for a typical gas mixture used in gas radiation detectors. The accuracy can be improved at the expense of computation time, the accuracy increasing approximately according to the square root of the computation time. The solution is general and allows the magnetic field to be at any angle to the electric field. The derived cross-section set for the gas, CF_4, is limited in accuracy by the inconsistency in the experimental data sets of drift velocity and diffusion coefficients. The gas data base for Magboltz [1] containing cross-sections for many other gases used in radiation detectors can also be used with this program.

References

[1] S.F. Biagi, Nucl. Instr. and Meth. A 283 (1989) 716.
[2] R. Veenhof, Garfield, A drift chamber simulation program, CERN Program Library, 1998.
[3] Maxwell Electric Field Simulator, ANSOFT Corporation.
[4] K.F. Ness, Phys. Rev. E 47 (1993) 327.
[5] K.F. Ness, J. Phys. D 27 (1994) 1848.
[6] I.D. Reid, Aust. J. Phys. 32 (1979) 231.
[7] G.W. Fraser, E. Mathieson, Nucl. Instr. and Meth. A 247 (1986) 544.
[8] H.R. Skullerud, J. Phys. D 1 (1968) 1567.

[9] S. Longo, M. Capitelli, Plasma Chem. Plasma Process. 14 (1993) 1.
[10] R. Kubo, Rep. Prog. Phys. 29 (1966) 255.
[11] A. Mann, F. Linder, J. Phys. B 25 (1992) 533.
[12] A. Mann, F. Linder, J. Phys. B 25 (1992) 545.
[13] L. Boesten, H. Tanaka, A. Kobayashi, M.A. Dillon, M. Kimura, J. Phys. B 25 (1992) 1607.
[14] L. Iga, M.V.V.S. Rao, S.K. Srivastava, J.C. Nogueira, Z. Phys. D 24 (1992) 111.
[15] R.K. Jones, J. Chem. Phys. 84 (1986) 813.
[16] M.A. Bruce, C.E. Ma, R.A. Bonham, Chem. Phys. Lett. 190 (1992) 285.
[17] R.A. Bonham, Jpn. J. Appl. Phys. 33 (1994) 4157.
[18] B. Schmidt, S. Polenz, Nucl. Instr. and Meth. A 273 (1988) 488.
[19] S.R. Hunter, J.G. Carter, L.G. Christophorou, Phys. Rev A 38 (1988) 58.
[20] Y. Nakamura, S. Tomizawa, Papers of Technical meeting of Electrical Discharges, ED-88-58, IEE, Japan 1988, p. 29.
[21] M.G. Curtis, I.C. Walker, K.J. Mathieson, J. Phys. D 21 (1988) 1271.
[22] M.S. Naidu, A.N. Prasad, J. Phys. D 5 (1972) 983.
[23] M. Shimozuma, H. Tagashira, H. Hasegawa, J. Phys. D 16 (1983) 971.
[24] J. Dutton, A. Goodings, A.K. Lucas, A.W. Williams J. Phys. D 20 (1987) 1322.
[25] B. Schmidt, J. Phys. B 24 (1991) 4809.
[26] Y.-H. Chang, U.J. Becker, B.R. Smith, C. Wang, Nucl. Instr. and Meth. A 339 (1994) 524.
[27] T. Kunst, B. Gotz, B. Schmidt, Nucl. Instr. and Meth. A 324 (1993) 127.
[28] O. Kiselev, O. Prokofiev, A. Vorobyov, Nucl. Instr. and Meth. A 367 (1995) 306.