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**THE MULTI-TERM BOLTZMANN EQUATION ANALYSIS AND MONTE
CARLO STUDY OF HYDRODYNAMIC AND NON-HYDRODYNAMIC
CHARGED PARTICLE SWARMS**

Thesis submitted by
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in February 2009

for the degree of Doctor of Philosophy
in the School of Engineering and Physical Science
James Cook University

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Saša Dujko,

27 February 2009.

ACKNOWLEDGMENTS

I would like to express my sincere and hearty gratitude to my supervisor Dr R D White for his guidance, encouragement, inspiration, and support that made this work possible. He has helped greatly and constantly in both my professional and personal development during my stay at the James Cook University in Australia. I wish also to express my appreciation to Dr K F Ness for the assistance he has offered me.

My associate supervisors throughout the course of this project have been Prof. R E Robson and Prof. Z Lj Petrović. To both I extend my sincere thanks and acknowledge their expertise, interest and helpful discussions.

I would also like to thank Dr Z M Raspopović for numerous discussions, suggestions and help.

I also like to thank the help of Z Todosijević in useful discussions about numerical calculations.

I wish to thank the staffs of School of Engineering and Physical Sciences of James Cook University for their encouragement and support. I am also indebted to the members of the Laboratory for Gaseous Electronics at the Institute of Physics in Belgrade for the constructive and fruitful discussions on the subject matter of the present work.

I would like to acknowledge the financial support of the Australian Government and James Cook University through the IPRS scholarship.

Finally, I am most indebted to my wife, my daughter, my parents, and my brother for their everlasting love, encouragement, patience, and support throughout the course of my education.

Abstract

The progress and further improvement of modern technology associated with the non-equilibrium magnetized plasma discharges require the most accurate modeling of charged particle transport under the influence of electric and magnetic fields in neutral gases. It is the aim of this Thesis to present a theoretical and numerical investigation of hydrodynamic and non-hydrodynamic charged particle swarms in neutral gases under the influence of dc and ac electric and magnetic fields with applications of non-equilibrium magnetized plasma discharges to plasma processing, gas laser discharges and drift chambers for detection particles in mind. Two complimentary techniques are developed: A time-dependent true multi-term solution of Boltzmann's equation and a Monte Carlo simulation technique, both adapted to consider both time-dependent hydrodynamic and steady state non-hydrodynamic conditions. The accuracy and generality of both techniques are established in their application to benchmark systems (existing and developed as part of the thesis) as well as the application to real gaseous systems.

Binary elastic, inelastic and non-conservative (attachment and electron impact ionization) collisions between the swarm particles and neutral gas molecules are considered. The angular dependence of the phase space distribution function in velocity space is represented in terms of an expansion in spherical harmonics. No restrictions are placed on the number of spherical harmonics in the polynomial expansion nor on the space and time-dependence of the phase space distribution function. In addition, there are no restrictions on the mass ratio between the swarm particle and neutral gas molecule (e.g., the present formalism is equally valid for electrons and ions) nor on the neutral gas temperature and cross sections. The speed dependence of the phase space distribution function is represented by an expansion in Sonine polynomials about a Maxwellian distribution function using a well-known two-temperature method. By doing so, the Boltzmann equation is decomposed into a hierarchy of coupled kinetic equations for tensorial expansion coefficients.

For time-dependent hydrodynamic regime, the space dependence of the phase space distribution function is represented in terms of powers of density gradient operator. A second order density gradient expansion was required to highlight the explicit modification of transport coefficients about by non-conservative collisional processes of attachment and electron impact ionization. Employing the implicit finite difference scheme for evaluation of the time-derivatives, the Boltzmann equation under conditions of time-dependent hydrodynamic regime is transformed into a hierarchy of doubly infinite coupled inhomogeneous matrix equations for the time-dependent moments. Truncation of both the Sonine polynomials and spherical harmonics results in a sparse system of coupled complex equations. This system of equations is solved using standard sparse inversion routines.

Under non-hydrodynamic conditions (such as those found in an idealized steady-state Townsend (SST) experiment) a density gradient expansion procedure is not valid and the space dependence of the phase space distribution function is retained explicitly throughout the entire decomposition process of the Boltzmann equation. For numerical discretization in configuration space the finite difference scheme and pseudo-spectral method are employed. Boundary conditions are

specified for swarms undergoing conservative collisions only and techniques for solving the resulting large system of algebraic complex equations are discussed. The explicit effects of ionization and attachment on the spatially resolved electron transport properties under non-hydrodynamic conditions are investigated by a Monte Carlo simulation technique. In particular, we identify the relations for the conversion of hydrodynamic transport properties to those found in an idealized steady-state Townsend experiment. Our Monte Carlo simulation code and sampling techniques appropriate to these experiments have provided us with a way to test these conversion formulae and their convergence.

For swarms moving in an unbounded gas under hydrodynamic conditions when non-conservative collisions are operative, we focus on two situations: (i) temporal relaxation of the electrons in dc electric and magnetic fields crossed at arbitrary angle; and (ii) time-dependent behavior of electron swarms in ac electric and magnetic fields crossed at arbitrary angle and at arbitrary phase difference. There are no restrictions on the field amplitudes nor on the frequency of the applied electric and magnetic fields. Recent studies on the temporal relaxation of electrons in gases are extended by overcoming the inherent inaccuracies of the two-term approximation for solving the Boltzmann equation and by addressing the temporal relaxation of spatial inhomogeneities through a study of the diffusion tensor. In the framework of ac studies, the variation of the electron transport coefficients with electric and magnetic field strengths, field frequency, phase difference between the fields and angle between the fields is addressed using physical arguments for certain model and real gases. A multitude of kinetic phenomena were observed that are generally inexplicable through the use of steady-state dc transport theory. Phenomena of significant note include the existence of transient negative diffusivity, time-resolved negative differential conductivity and anomalous anisotropic diffusion. Most notably, a proposed new mechanism for collisional heating in inductively coupled plasmas has emerged from this thesis. It is shown that the synergism of temporal non-locality and cyclotron resonance effect under conditions of time-dependent, high frequency electric and magnetic fields can be used to pump the energy into the swarm. In particular, it is demonstrated that the magnetic field amplitude, phase-difference between the fields and field frequency can be tuned to exploit/control this phenomenon.

The synergism of magnetic field and non-conservative collisions on spatial relaxation of a swarm of charged particles in an idealized SST experiment is investigated. Results are presented for electrons in varying configurations of dc electric and magnetic fields for certain model and real gases. It is found that the spatial relaxation characteristics including the type of relaxation (monotonic/oscillatory), the relaxation length and period of oscillations can be controlled either by the variation of the magnetic field strengths or by the angles between the fields.

Contents

1	Introduction	1
1.1	Motivation and aims	1
1.2	Nature of the problem and theoretical methods employed	5
1.3	Some factors in the historical development of the Boltzmann equation analysis under hydrodynamic conditions	8
1.3.1	Swarms in neutral gases under the influence of dc electric field	8
1.3.2	Swarms in neutral gases under the influence of dc electric and magnetic fields	14
1.3.3	Temporal relaxation processes of electron swarms in dc electric and magnetic fields	17
1.3.4	Swarms in neutral gases under the influence of ac electric field	21
1.4	Some factors in the historical development of the Boltzmann equation analysis under non-hydrodynamic conditions	27
1.4.1	Non-hydrodynamic phenomena in transport of charged particles	27
1.4.2	Techniques of solving the Boltzmann equation under non-hydrodynamic conditions	28
1.5	A brief sketch of Monte Carlo simulation technique under hydrodynamic and non-hydrodynamic conditions	34
1.6	Scope and structure of the thesis	40
2	Spherical harmonic decomposition of the Boltzmann equation	43
2.1	Introduction	43
2.2	Mathematical background: Algebra of irreducible tensors	44
2.3	Hydrodynamic and non-hydrodynamic regimes	47

2.3.1	The time-dependent hydrodynamic regime and definitions of transport coefficients	48
2.3.2	Non-hydrodynamic regime and definitions of transport properties	50
2.4	Spherical harmonics decomposition of the Boltzmann equation	52
2.4.1	Expansion of the velocity distribution function	52
2.4.2	Boltzmann equation decomposed in a spherical harmonics basis	52
2.5	Time-dependent hydrodynamic regime	55
2.5.1	The density gradient expansion in the time-dependent hydrodynamic regime	55
2.5.2	Hierarchy of kinetic equations	57
2.5.3	Change in the form of hierarchy equations through inclusion of the time-dependent magnetic field	60
2.5.4	Transport coefficients and transport properties in the time-dependent hydrodynamic regime	62
2.5.4.1	Transport coefficients	62
2.5.4.2	Transport properties	64
2.6	Steady-state non-hydrodynamic regime	67
2.6.1	Transport properties in the non-hydrodynamic regime	68
3	The kinetic equations in a Sonine polynomial basis	69
3.1	Introduction	69
3.2	Time-dependent hydrodynamic regime	70
3.2.1	Representation of the speed dependence in terms of Sonine polynomials .	70
3.2.2	Hierarchy of kinetic equations in a Sonine polynomial basis	71
3.2.3	Transport coefficients, properties and distribution function	73
3.2.4	Temporal discretization of the hierarchy of kinetic equations	76
3.3	Steady-state non-hydrodynamic regime	77
3.3.1	Transport properties in the non-hydrodynamic regime	78
3.4	Treatment of the collision operator	78
3.4.1	Conservative collision matrix	79
3.4.2	Non-conservative collision matrix	81
3.4.2.1	Attachment collision matrix	81

3.4.2.2	Ionization collision matrix	82
4	Numerical considerations of the decomposed Boltzmann equation solutions	84
4.1	Numerical solutions of the hierarchy of moment equations in the time-dependent hydrodynamic regime	84
4.1.1	The convergence criterion and choice of basis parameters	86
4.2	Numerical solution of the moment equations in the steady-state non-hydrodynamic regime	89
4.2.1	Boundary conditions	89
4.2.2	Treatment of spatial derivatives using pseudo-spectral and finite difference methods	90
4.2.2.1	Pseudo-spectral method	91
4.2.2.2	Finite difference approximation	94
4.2.3	Truncation, convergence and choice of basis temperature	97
5	Monte Carlo simulation technique	98
5.1	Introduction	98
5.2	Overview of the Monte Carlo codes	100
5.3	Random number generator	100
5.4	Simulation of an electron path in electric and magnetic fields	101
5.5	Determining the probability and nature of the collisions	103
5.6	Determining the scattering parameters	105
5.7	Sampling techniques under hydrodynamic and non-hydrodynamic conditions . .	106
5.7.1	General considerations: distribution functions, macroscopic quantities and hydrodynamic regime	106
5.7.2	The calculation of bulk and flux transport coefficients	108
5.7.3	Transport under SST conditions	109
5.7.3.1	Sampling of spatially resolved transport data	110
5.7.4	On the calculation of coefficients in the hydrodynamic expansion	112
6	Benchmark calculation of electron transport in dc electric and magnetic fields crossed at arbitrary angle	114
6.1	Introduction	114

6.2	The Reid ramp model	116
6.3	The Ionization model of Lucas and Saelee	117
6.3.1	Mean energy and ionization rate	119
6.3.2	Drift speed, drift velocity components and gradient energy vector components	120
6.3.3	Diagonal elements of the diffusion tensor	124
6.3.4	Off-diagonal elements of the diffusion tensor	128
6.3.5	The diagonal elements of the temperature tensor	130
6.4	The modified attachment model of Ness and Robson	131
6.4.1	Mean energy and attachment rate	132
6.4.2	Drift speed, drift velocity components and gradient energy vector components	133
6.4.3	Diagonal elements of the diffusion tensor	135
6.4.4	Off-diagonal elements of the diffusion tensor	139
6.4.5	The diagonal elements of the temperature tensor	139
6.5	Two term approximation vs multi-term calculations and validity of Legendre polynomial expansions	140
7	Temporal relaxation of electron swarm in dc electric and magnetic fields crossed at arbitrary angle	147
7.1	Introduction	147
7.2	Inelastic system: Reid ramp model	148
7.2.1	Transient negative electron diffusivity	152
7.2.2	The effect of angle between the fields on the temporal relaxation profiles .	154
7.3	The ionization model of Lucas and Saelee	160
7.3.1	The effect of the ionization processes	162
7.3.2	The effect of the angle between the fields on the temporal relaxation profiles	170
7.3.3	The influence of the reduced electric field on the temporal relaxation profiles	174
7.4	Temporal relaxation of electrons in real gases	180
7.4.1	Preliminaries	180
7.4.2	Temporal relaxation of electrons in CO ₂	182
7.4.3	Temporal relaxation of electrons in CO ₂ -argon mixtures	184

8	Electron swarms in ac electric and magnetic fields	188
8.1	Introduction	188
8.2	Traditional description of the temporal profiles of the transport properties	191
8.3	Electron swarms in CF ₄ and argon-CF ₄ mixtures in ac electric fields	193
8.3.1	Preliminaries	193
8.3.2	Electron transport properties in CF ₄	194
8.3.3	Electron transport properties in CF ₄ -argon mixtures	202
8.4	The influence of magnetic field on the electron transport properties	207
8.4.1	Benchmark comparison: Reid ramp model	207
8.4.2	The effects of the magnetic field strength on the electron transport properties in ac electric and magnetic fields	209
8.4.3	The effects of the phase-difference between the fields on the electron transport properties in ac electric and magnetic fields	219
8.4.4	The effects of the field configuration on the electron transport properties in rf electric and magnetic fields	224
8.4.5	The effects of non-conservative collisions on the electron transport properties in rf electric and magnetic fields	230
8.4.5.1	The ionization model of Lucas and Saelee	230
8.4.5.2	The modified attachment model of Ness and Robson	239
8.4.6	The collisional heating mechanism in rf electric and magnetic fields	246
8.4.7	The validity of the two-term approximation in rf electric and magnetic fields	251
9	Spatial relaxation of electron swarm in dc electric and magnetic fields crossed at arbitrary angle	255
9.1	Introduction	255
9.2	Spatial relaxation of electron swarms in dc electric fields	256
9.2.1	Inelastic system: Step model	256
9.2.2	The ionization model of Lucas and Saelee	259
9.2.3	The modified attachment model of Ness and Robson	263
9.2.4	Real gases: argon, CF ₄ and argon-CF ₄ mixture	264
9.3	The effects of magnetic field on the spatial relaxation profiles	268
9.3.1	Inelastic systems: Step and conservative Lucas-Saelee ionization models	268

9.3.2	The Lucas-Saelee ionization model and Ness-Robson modified attachment model	272
10	Concluding remarks	278
A	Benchmark Calculations: The ionization model of Lucas and Saelee	281
B	Benchmark Calculations: The modified attachment model of Ness and Robson	288

List of Figures

2.1	Schematic representation of the idealized steady-state Townsend experiment. Charged particles emitted at a constant rate from an infinite plane source at $z = z_0$ interact with the background neutral gas under static external electric and magnetic fields and evolve downstream $z \geq z_0$	51
4.1	The variation of the basis temperature of 1000 K as a function of number of iterations.	88
5.1	Comparison between electron orbits in uniform, static magnetic field obtained via different techniques for solving the equation of motion of a single electron.	103
6.1	Variation of the mean energy (a) and ionization rate (b) as a function of B/n_0 and ψ for the ionization model of Lucas and Saelee. The solid, dashed and dotted lines (black: 100 Hx; red: 200 Hx; blue: 1000 Hx) represent the mean energies for $F = 0$, $F = 0.5$ and $F = 1$, respectively.	120
6.2	Variation of the drift speed (a) and z -drift velocity component (b) as a function of B/n_0 and ψ for the ionization model of Lucas and Saelee. The solid lines (black: 100 Hx; red: 200 Hx; blue: 1000 Hx) represent the flux values while the dashed and dotted lines represent the bulk values for $F = 0.5$ and $F = 1$, respectively.	121
6.3	Variation of the x - (a) and y - (b) drift velocity components as a function of B/n_0 and ψ for the ionization model of Lucas and Saelee for the same conditions as those in Fig. 6.2.	122
6.4	Variation of the y - and z -components of the gradient energy vector as a function of B/n_0 and ψ for the ionization model of Lucas and Saelee for the same conditions as those in Fig. 6.1.	122
6.5	Variation of the x -component of the gradient energy vector as a function of B/n_0 and ψ for the ionization model of Lucas and Saelee for the same conditions as those in Fig. 6.1.	123

6.6	Variation of the flux components of $n_0 D_{xx}$ (a) and $n_0 D_{zz}$ (b) as a function of B/n_0 and ψ for the ionization model of Lucas and Saelee. The solid, dashed and dotted lines (black: 100 Hx; red: 500 Hx; blue: 1000 Hx) represent $n_0 D_{xx}$ and $n_0 D_{zz}$ for $F = 0$, $F = 0.5$ and $F = 1$, respectively.	125
6.7	Variation of the flux components of $n_0 D_{yy}$ as a function of B/n_0 and ψ for the ionization model of Lucas and Saelee for the same conditions as those in Fig. 6.6.	126
6.8	The percentage difference between the bulk and flux values of $n_0 D_{yy}$ and $n_0 D_{zz}$ as a function of ψ for B/n_0 of 100, 200 and 500 Hx.	127
6.9	The percentage difference between the bulk and flux values of $n_0 D_{xx}$ as a function of ψ for B/n_0 of 100, 200 and 500 Hx.	127
6.10	Variation of the off-diagonal elements of the diffusion tensor as a function of B/n_0 and ψ for the ionization model of Lucas and Saelee for the same conditions as those in Fig. 6.6.	129
6.11	Variation of the Hall diffusion coefficient as a function of B/n_0 for the ionization model of Lucas and Saelee.	129
6.12	Variation of the diagonal elements of the temperature tensor as a function of B/n_0 and ψ for the ionization model of Lucas and Saelee for the same conditions as those in Fig. 6.1.	130
6.13	Variation of the mean energy and attachment rate as a function of B/n_0 and ψ for the modified attachment model of Ness and Robson. Black, red, green and blue lines (solid lines: 100 Hx; dashed lines: 200 Hx; dotted lines: 1000 Hx) represent the mean energies for conservative (no attachment) case, non-conservative cases when the attachment cross section is directly proportional to the electron velocity with the attachment amplitudes $a = 0.3$ and $a = 0.5$, and non-conservative case when the electron attachment is inversely proportional to the electron energy, respectively.	133
6.14	Variation of the drift speed and W_z as a function of B/n_0 and ψ for the modified attachment model of Ness and Robson. Black lines represent the flux values while red, green and blue lines represent the bulk values when the attachment cross section is directly proportional to the electron velocity with the attachment amplitudes $a = 0.3$ and $a = 0.5$, and when the electron attachment is inversely proportional to the electron energy, respectively (solid lines: 100 Hx; dashed lines: 200 Hx; dotted lines: 1000 Hx).	134
6.15	Variation of W_x and W_y drift velocity components as a function of B/n_0 and ψ for the modified attachment model of Ness and Robson for the same conditions as in Fig. 6.14	135

6.16	Variation of the y - (a) and z - (b) components of the gradient energy vector as a function of B/n_0 and ψ for the modified attachment model of Ness and Robson for the same conditions as in Fig. 6.13.	136
6.17	Variation of the flux components of $n_0 D_{xx}$ (a) and $n_0 D_{zz}$ (b) as a function of B/n_0 and ψ for the modified attachment model of Ness and Robson for the same conditions as in Fig. 6.13.	136
6.18	Variation of the flux component of $n_0 D_{yy}$ as a function of B/n_0 and ψ for the modified attachment model of Ness and Robson for the same conditions as in Fig. 6.13.	137
6.19	The percentage difference between the bulk and flux values of $n_0 D_{yy}$ (a) and $n_0 D_{zz}$ (b) as a function of ψ for B/n_0 of 100, 200 and 500 Hx for the modified attachment model of Ness and Robson.	137
6.20	Variation of the off-diagonal elements $D_{xy}, D_{yx}, D_{xz}, D_{zx}$ as a function of B/n_0 and ψ for the modified attachment model of Ness and Robson for the same conditions as in Fig. 6.13.	138
6.21	Variation of the off-diagonal elements of D_{yz}, D_{zy} as a function of B/n_0 and ψ for the modified attachment model of Ness and Robson for the same conditions as in Fig. 6.13.	139
6.22	Variation of the diagonal elements of the temperature tensor as a function of B/n_0 and ψ for the modified attachment model of Ness and Robson for the same conditions as in Fig. 6.13.	140
6.23	The percentage difference between two-term and multi-term results for the mean energy, ionization rate and z -component of the gradient energy vector as a function of ψ for the ionization model of Lucas and Saelee (black line: $E/n_0 = 100$ Td; red line: $E/n_0 = 200$ Td).	141
6.24	The percentage difference between two-term and multi-term results for the drift velocity components as a function of ψ for the ionization model of Lucas and Saelee. The solid lines represent the flux values while the dashed lines represent the bulk values (black line: $E/n_0 = 100$ Td; red line: $E/n_0 = 200$ Td).	142
6.25	The percentage difference between two-term and multi-term results for the diagonal elements of the diffusion tensor as a function of ψ for the ionization model of Lucas and Saelee. The solid lines represent the flux values while the dashed lines represent the bulk values (black line: $E/n_0 = 100$ Td; red line: $E/n_0 = 200$ Td).	143
6.26	The percentage difference between two-term and multi-term results for the diagonal elements of the temperature tensor as a function of ψ for the ionization model of Lucas and Saelee (black line: $E/n_0 = 100$ Td; red line: $E/n_0 = 200$ Td).	144

6.27	The percentage difference between results for the mean energy, ionization rate and z -component of the gradient energy vector obtained for the $m_{\max} = 1$ and 5 truncation ($l_{\max} = 5$) as a function of ψ for the ionization model of Lucas and Saelee (black line: $E/n_0 = 100$ Td; blue line: $E/n_0 = 200$ Td).	144
6.28	The percentage difference between results for the drift velocity components obtained for the $m_{\max} = 1$ and 5 truncation ($l_{\max} = 5$) as a function of ψ for the ionization model of Lucas and Saelee. The solid lines represent the flux values while the dashed lines represent the bulk values (black line: $E/n_0 = 100$ Td; blue line: $E/n_0 = 200$ Td).	145
6.29	The percentage difference between results for the diagonal elements of the diffusion tensor obtained for the $m_{\max} = 1$ and 5 truncation ($l_{\max} = 5$) as a function of ψ for the ionization model of Lucas and Saelee. The solid lines represent the flux values while the dashed lines represent the bulk values (black line: $E/n_0 = 100$ Td; blue line: $E/n_0 = 200$ Td).	146
6.30	The percentage difference between results for the diagonal elements of the temperature tensor obtained for the $m_{\max} = 1$ and 5 truncation ($l_{\max} = 5$) as a function of ψ for the ionization model of Lucas and Saelee (black line: $E/n_0 = 100$ Td; blue line: $E/n_0 = 200$ Td).	146
7.1	Comparison of the reduced cyclotron period for various B/n_0 (solid horizontal lines) with the reduced timescales for momentum and energy relaxation as a function of energy.	150
7.2	Temporal relaxation of the mean energy, drift velocity components and diagonal elements of the diffusion tensor for various applied magnetic fields in a crossed field configuration for Reid ramp model (solid black lines: Multi term Boltzmann code; dashed colored lines: Monte Carlo code)	151
7.3	Temporal relaxation of the diagonal elements of the temperature tensor for various applied magnetic fields in a crossed field configuration for Reid ramp model.	153
7.4	Temporal relaxation of the mean energy, drift speed and z -component of the gradient energy vector for various angles between the fields (black lines: 0° ; red lines: 30° ; green lines: 60° ; blue lines: 90°) and B/n_0 of 100 Hx (the first row) and B/n_0 of 1000 Hx (the second row) for Reid ramp model.	154
7.5	Temporal relaxation of the drift velocity components for the same conditions as in figure 7.4.	155
7.6	Temporal relaxation of the diagonal elements of the diffusion tensor for the same conditions as in figure 7.4.	155
7.7	Temporal relaxation of $n_0 D_{xx}$ for the same conditions as in figure 7.4.	157

7.8	Temporal relaxation of the diagonal elements of the diffusion tensor for B/n_0 of 100 and 1000 Hx and ψ of 30° and 60° for Reid ramp model (color lines: multi-term calculations; black lines: two-term approximation).	159
7.9	Comparison of the reduced cyclotron period for various B/n_0 (solid horizontal lines) with the reduced timescales for momentum and energy relaxation as a function of energy for the ionization model of Lucas and Saelee.	161
7.10	Temporal relaxation of the mean energy as a function of B/n_0 and fixed ψ of 75° for the ionization model of Lucas and Saelee (black line: $F = 0$, red line: $F = 0.5$, blue line: $F = 1$).	163
7.11	Temporal relaxation of the ionization rate as a function of B/n_0 and fixed ψ of 75° for the ionization model of Lucas and Saelee (black line: $F = 0$, red line: $F = 0.5$, blue line: $F = 1$).	163
7.12	Temporal relaxation of W_x as a function of B/n_0 and fixed ψ of 75° for the ionization model of Lucas and Saelee.	164
7.13	Temporal relaxation of W_y as a function of B/n_0 and fixed ψ of 75° for the ionization model of Lucas and Saelee (black line: $F = 0$, red line: $F = 0.5$, blue line: $F = 1$).	164
7.14	Temporal relaxation of W_z as a function of B/n_0 and fixed ψ of 75° for the ionization model of Lucas and Saelee (black line: $F = 0$, red line: $F = 0.5$, blue line: $F = 1$).	165
7.15	Temporal relaxation of γ_x as a function of B/n_0 and fixed ψ of 75° for the ionization model of Lucas and Saelee (black line: $F = 0$, red line: $F = 0.5$, blue line: $F = 1$).	166
7.16	Temporal relaxation of γ_y as a function of B/n_0 and fixed ψ of 75° for the ionization model of Lucas and Saelee (black line: $F = 0$, red line: $F = 0.5$, blue line: $F = 1$).	166
7.17	Temporal relaxation of γ_z as a function of B/n_0 and fixed ψ of 75° for the ionization model of Lucas and Saelee (black line: $F = 0$, red line: $F = 0.5$, blue line: $F = 1$).	167
7.18	Temporal relaxation of $n_0 D_{xx}$ as a function of B/n_0 and fixed ψ of 75° for the ionization model of Lucas and Saelee (full lines: flux; dashed lines: bulk).	168
7.19	Temporal relaxation of $n_0 D_{yy}$ as a function of B/n_0 and fixed ψ of 75° for the ionization model of Lucas and Saelee (full lines: flux; dashed lines: bulk).	168
7.20	Temporal relaxation of $n_0 D_{zz}$ as a function of B/n_0 and fixed ψ of 75° for the ionization model of Lucas and Saelee (full lines: flux; dashed lines: bulk).	169

7.21	Temporal relaxation of the mean energy (a) and ionization rate (b) as a function of ψ and fixed B/n_0 of 500 Hx for the ionization model of Lucas and Saelee.	170
7.22	Temporal relaxation of W_x and γ_x as a function of ψ and fixed B/n_0 of 500 Hx for the ionization model of Lucas and Saelee.	171
7.23	Temporal relaxation of W_y and γ_y as a function of ψ and fixed B/n_0 of 500 Hx for the ionization model of Lucas and Saelee.	171
7.24	Temporal relaxation of W_z and γ_z as a function of ψ and fixed B/n_0 of 500 Hx for the ionization model of Lucas and Saelee.	172
7.25	Temporal relaxation of D_{yy} and D_{zz} as a function of ψ and fixed B/n_0 of 500 Hx for the ionization model of Lucas and Saelee.	173
7.26	Temporal relaxation of the mean energy and ionization rate as a function of E/n_0 for B/n_0 of 500 Hx and ψ of 60° for the ionization model of Lucas and Saelee (black line: 10 Td; red line: 20 Td; green line: 30 Td; blue line: 40 Td).	175
7.27	Temporal relaxation of W_x and W_y as a function of E/n_0 for fixed B/n_0 of 500 Hx and for fixed ψ of 60° for the ionization model of Lucas and Saelee (black line: 10 Td; red line: 20 Td; green line: 30 Td; blue line: 40 Td).	176
7.28	Temporal relaxation of W_z as a function of E/n_0 for fixed B/n_0 of 500 Hx and for fixed ψ of 60° for the ionization model of Lucas and Saelee (black line: 10 Td; red line: 20 Td; green line: 30 Td; blue line: 40 Td).	176
7.29	Temporal relaxation of the gradient energy vector components as a function of E/n_0 for fixed B/n_0 of 500 Hx and for fixed ψ of 60° for the ionization model of Lucas and Saelee (black line: 10 Td; red line: 20 Td; green line: 30 Td; blue line: 40 Td).	177
7.30	Temporal relaxation of D_{xx} as a function of E/n_0 for fixed B/n_0 of 500 Hx and for fixed ψ of 60° for the ionization model of Lucas and Saelee (black line: 10 Td; red line: 20 Td; green line: 30 Td; blue line: 40 Td).	178
7.31	Temporal relaxation of D_{yy} and D_{zz} as a function of E/n_0 for fixed B/n_0 of 500 Hx and for fixed ψ of 60° for the ionization model of Lucas and Saelee (black line: 10 Td; red line: 20 Td; green line: 30 Td; blue line: 40 Td).	179
7.32	Electron impact cross-sections for (a) carbon dioxide (Bulos and Phelps, 1976) and (b) argon ((Hayashi, 1992); Ness and Makabe (2000)) used in this study. . .	180
7.33	Comparison of the reduced cyclotron period for various B/n_0 (solid horizontal lines) with the reduced timescales for momentum and energy relaxation as a function of energy for (a) carbon dioxide and (b) argon.	181

7.34	Temporal relaxation of the mean energy (a) and longitudinal drift velocity component (b) for various angles between the fields for electrons in CO ₂ at E/n_0 of 12 Td and B/n_0 500 Hx. (dashed lines: two-term approximation; full lines: multi-term theory)	182
7.35	Temporal relaxation of the $n_0 D_{yy}$ and $n_0 D_{zz}$ for various angles between the fields for electrons in CO ₂ at E/n_0 of 12 Td and B/n_0 500 Hx. (dashed lines: two-term approximation; full lines: multi-term theory)	183
7.36	Temporal relaxation of the $n_0 D_{zx}$ and $n_0 D_{yz}$ for various angles between the fields for electrons in CO ₂ at E/n_0 of 12 Td and B/n_0 100 Hx. (dashed lines: two-term approximation; full lines: multi-term theory)	184
7.37	Temporal relaxation of the mean energy (a) and longitudinal drift velocity component (b) for various angles between the fields for electrons in CO ₂ -argon mixtures at E/n_0 of 12 Td and B/n_0 500 Hx.	185
7.38	Temporal relaxation of W_x (a) and W_y (b) for various angles between the fields for electrons in CO ₂ -argon mixtures at E/n_0 of 12 Td and B/n_0 500 Hx.	185
7.39	Temporal relaxation of $n_0 D_{yy}$ (a) and $n_0 D_{zz}$ (b) for various angles between the fields for electrons in CO ₂ -argon mixtures at E/n_0 of 12 Td and B/n_0 500 Hx.	186
7.40	Temporal relaxation of $n_0 D_{xx}$ for various angles between the fields for electrons in CO ₂ -argon mixtures at E/n_0 of 12 Td and B/n_0 500 Hx.	186
8.1	(a) Electron impact cross-section for CF ₄ (Kurihara <i>et al.</i> , 2000) includes elastic momentum transfer (1), three vibrational (2-4) and one electronic excitation cross section (5), attachment cross section (6), seven dissociative ionization cross sections (7-13) and three cross sections for neutral dissociation (14-16); (b) Energy-resolved frequencies for momentum $\nu_e^m(\epsilon)$ and energy $\nu_e(\epsilon)$ relaxation of electrons at the pressure of 1 Torr.	194
8.2	Temporal profiles of the mean energy for electrons in CF ₄ under the influence of an electric field of the form $E(t)/n_0 = 100 \cos(2\pi ft)$ Td for various applied frequencies.	195
8.3	Temporal profiles of the gradient energy parameter for electrons in CF ₄ under the influence of an electric field of the form $E(t)/n_0 = 100 \cos(2\pi ft)$ Td for various applied frequencies.	196
8.4	Temporal profiles of the drift velocity for electrons in CF ₄ under the influence of an electric field of the form $E(t)/n_0 = 100 \cos(2\pi ft)$ Td for various applied frequencies.	197
8.5	Temporal profiles of the diffusion coefficients for electrons in CF ₄ under the influence of an electric field of the form $E(t)/n_0 = 100 \cos(2\pi ft)$ Td for various applied frequencies.	198

8.6	The spatially dependent average energies (a) and average velocities (b) during one half of the period of the field at different phases as indicated on the graph.	200
8.7	The spatial distributions of the forward (a) and backward (b) moving electrons during one half of the period of the field at different phases as indicates on the graph.	201
8.8	Comparison of the two-term and multi-term profiles of the diffusion coefficients for electrons in CF_4 at various field frequencies.	202
8.9	Temporal variation of the mean energy with the frequency for various CF_4 -argon mixtures.	203
8.10	Temporal variation of the gradient energy parameter with the frequency for various CF_4 -argon mixtures.	204
8.11	Temporal variation of the reaction rate with the field frequency for various CF_4 -argon mixtures.	205
8.12	Temporal variation of the drift speed with the frequency for various CF_4 -argon mixtures.	205
8.13	Temporal variation of the longitudinal diffusion coefficient with the frequency for various CF_4 -argon mixtures.	206
8.14	Temporal variation of the transverse diffusion coefficient with the frequency for various CF_4 -argon mixtures.	206
8.15	Comparison of the Boltzmann equation (black) and Monte Carlo (red) results for ε over a range of applied field frequencies for the Reid ramp model.	208
8.16	Comparison of the Boltzmann equation (black) and Monte Carlo (red) results for W_z and W_x over a range of applied field frequencies for the Reid ramp model.	209
8.17	Comparison of the Boltzmann equation (black) and Monte Carlo (red) results for $n_0 D_{zz}$ and $n_0 D_{xx}$ over a range of applied field frequencies for the Reid ramp model.	209
8.18	The variation of the temporal profiles of the mean energy with B_0/n_0 in a crossed field configuration for various ω/n_0 for the Reid ramp model. The amplitude of electric field is 12 Td.	210
8.19	The variation of the temporal profiles of the longitudinal drift velocity component with B_0/n_0 in a crossed field configuration for various ω/n_0 for the Reid ramp model. The amplitude of electric field is 12 Td.	211
8.20	The variation of the temporal profiles of the transverse drift velocity component with B_0/n_0 in a crossed field configuration for various ω/n_0 for the Reid ramp model. The amplitude of electric field is 12 Td.	212

8.21	The variation of the temporal profiles of the longitudinal diffusion coefficient $n_0 D_{zz}$ with B_0/n_0 in a crossed field configuration for various ω/n_0 for the Reid ramp model. The amplitude of electric field is 12 Td.	214
8.22	The variation of the temporal profiles of the transverse diffusion coefficient $n_0 D_{yy}$ with B_0/n_0 in a crossed field configuration for various ω/n_0 for the Reid ramp model. The amplitude of electric field is 12 Td.	215
8.23	The variation of the temporal profiles of the transverse diffusion coefficient $n_0 D_{xx}$ with B_0/n_0 in a crossed field configuration for various ω/n_0 for the Reid ramp model. The amplitude of electric field is 12 Td.	216
8.24	The cycle-averaged values of the diagonal elements of the diffusion tensor as a function of B_0/n_0 in a crossed field configuration for various ω/n_0 for the Reid ramp model. The amplitude of electric field is 12 Td.	217
8.25	The variation of the temporal profiles of the Hall diffusion coefficient with B_0/n_0 in a crossed field configuration for various ω/n_0 for the Reid ramp model. The amplitude of electric field is 12 Td.	218
8.26	Contour plots of the temporal variation of the spatially homogeneous energy distribution function with B_0/n_0 ((a) black line: $B_0/n_0 = 0$ Hx; red line: $B_0/n_0 = 200$ Hx and (b) blue line: $B_0/n_0 = 500$ Hx) in a crossed field configuration for Reid's ramp model. The amplitude of electric field is 12 Td.	218
8.27	The 3-dimensional plots of the temporal profiles of the mean energy as a function of the phase-difference θ between the fields for different B_0/n_0 for the Reid ramp model.	219
8.28	The 3-dimensional plots of the longitudinal drift velocity component as a function of the phase-difference θ between the fields for different B_0/n_0 for the Reid ramp model.	220
8.29	The 3-dimensional plots of the transverse drift velocity component along the $\mathbf{E} \times \mathbf{B}$ direction as a function of the phase-difference θ between the fields for different B_0/n_0 for the Reid ramp model.	221
8.30	The 3-dimensional plots of the $n_0 D_{xx}$ as a function of the phase-difference θ between the fields for different B_0/n_0 for the Reid ramp model.	222
8.31	The 3-dimensional plots of the $n_0 D_{yy}$ as a function of the phase-difference θ between the fields for different B_0/n_0 for the Reid ramp model.	222
8.32	The 3-dimensional plots of the $n_0 D_{zz}$ as a function of the phase-difference θ between the fields for different B_0/n_0 for the Reid ramp model.	223
8.33	The 3-dimensional plots of the $n_0 D_{\text{Hall}}$ as a function of the phase-difference θ between the fields for different B_0/n_0 for the Reid ramp model.	224

8.34	The 3-dimensional plots of the mean energy as a function of the angle between the fields for ac magnetic field amplitude $B_0/n_0 = 1000$ Hx and dc magnetic field $B/n_0 = 1000$ Hx for the Reid ramp model.	225
8.35	The 3-dimensional plots of the longitudinal drift velocity component W_x as a function of the angle between the fields for ac magnetic field amplitude $B_0/n_0 = 1000$ Hx and dc magnetic field $B/n_0 = 1000$ Hx for the Reid ramp model.	226
8.36	The 3-dimensional plots of W_y as a function of the angle between the fields for ac magnetic field amplitude $B_0/n_0 = 1000$ Hx and dc magnetic field $B/n_0 = 1000$ Hx for the Reid ramp model.	227
8.37	The 3-dimensional plots of W_z as a function of the angle between the fields for ac magnetic field amplitude $B_0/n_0 = 1000$ Hx and dc magnetic field $B/n_0 = 1000$ Hx for the Reid ramp model.	227
8.38	The 3-dimensional plots of the diffusion coefficient $n_0 D_{xx}$ as a function of the angle between the fields for ac magnetic field amplitude $B_0/n_0 = 1000$ Hx and dc magnetic field $B/n_0 = 1000$ Hx for the Reid ramp model.	228
8.39	The 3-dimensional plots of the diffusion coefficient $n_0 D_{yy}$ as a function of the angle between the fields for ac magnetic field amplitude $B_0/n_0 = 1000$ Hx and dc magnetic field $B/n_0 = 1000$ Hx for the Reid ramp model.	229
8.40	The 3-dimensional plots of the diffusion coefficient $n_0 D_{zz}$ as a function of the angle between the fields for ac magnetic field amplitude $B_0/n_0 = 1000$ Hx and dc magnetic field $B/n_0 = 1000$ Hx for the Reid ramp model.	229
8.41	Temporal profiles of the mean energy as a function of the magnetic field amplitude and phase difference between the fields for the ionization model of Lucas and Saelee. The solid, dashed and dotted lines (black line: $B_0/n_0 = 0$ Hx; red line: $B_0/n_0 = 100$ Hx; green line: $B_0/n_0 = 200$ Hx; blue line: $B_0/n_0 = 500$ Hx; pink line: $B_0/n_0 = 1000$ Hx) represent the mean energy for $F = 0$, $F = 0.5$ and $F = 1$, respectively.	231
8.42	The 3-dimensional plot of the ionization rate as a function of the phase difference θ for B_0/n_0 of 200 Hx for the ionization model of Lucas and Saelee. The parameter F is set to 0.5.	232
8.43	Temporal profiles of the bulk and flux longitudinal drift velocity components W_z as a function of the magnetic field amplitude and phase difference between the fields for the ionization model of Lucas and Saelee. The solid, dashed and dotted lines (black line: $B_0/n_0 = 0$ Hx; red line: $B_0/n_0 = 100$ Hx; green line: $B_0/n_0 = 200$ Hx; blue line: $B_0/n_0 = 500$ Hx; pink line: $B_0/n_0 = 1000$ Hx) represent the flux W_z -temporal profiles, the bulk W_z -temporal profiles for $F = 0.5$ and the bulk W_z -temporal profiles for $F = 1$, respectively.	233

8.44	Temporal profiles of the flux drift velocity component W_x as a function of the magnetic field amplitude and phase difference between the fields for the ionization model of Lucas and Saelee (red line: $B_0/n_0 = 100$ Hx; $B_0/n_0 = 200$ Hx; $B_0/n_0 = 500$ Hx; $B_0/n_0 = 1000$ Hx).	234
8.45	Temporal profiles of the z -component of the energy gradient vector as a function of the magnetic field amplitude and phase difference between the fields for the ionization model of Lucas and Saelee for the same conditions as in figure 8.42. . .	235
8.46	Temporal profiles of the x -component of the gradient energy vector as a function of the magnetic field amplitude and phase difference between the fields for the ionization model of Lucas and Saelee for the same conditions as in figure 8.42. . .	236
8.47	Temporal profiles of the flux longitudinal diffusion coefficient $n_0 D_{zz}$ as a function of the magnetic field amplitude and phase difference between the fields for the ionization model of Lucas and Saelee for the same conditions as in figure 8.42. . .	237
8.48	Temporal profiles of the flux transverse diffusion coefficient $n_0 D_{yy}$ as a function of the magnetic field amplitude and phase difference between the fields for the ionization model of Lucas and Saelee for the same conditions as in figure 8.42. . .	237
8.49	Temporal profiles of the bulk and flux longitudinal diffusion coefficient $n_0 D_{zz}$ as a function of the magnetic field amplitude and phase difference between the fields for the ionization model of Lucas and Saelee. The solid lines (black line: $B_0/n_0 = 0$ Hx; red line: $B_0/n_0 = 100$ Hx; green line: $B_0/n_0 = 200$ Hx; blue line: $B_0/n_0 = 500$ Hx; pink line: $B_0/n_0 = 1000$ Hx) represent the flux profiles while the dashed lines represent the bulk for $F = 0.5$	238
8.50	Temporal profiles of the bulk and flux transverse diffusion coefficient $n_0 D_{xx}$ as a function of the magnetic field amplitude and phase difference between the fields for the ionization model of Lucas and Saelee for the same conditions as in figure 8.49.	239
8.51	Temporal profiles of the mean energy as a function of the magnetic field amplitude and phase difference between the fields for the modified attachment model of Ness and Robson. The solid, dashed and dotted lines (black line: $B_0/n_0 = 0$ Hx; red line: $B_0/n_0 = 100$ Hx; green line: $B_0/n_0 = 200$ Hx; blue line: $B_0/n_0 = 500$ Hx; pink line: $B_0/n_0 = 1000$ Hx) represent the mean energy for conservative (no attachment) case, $p = 0.5$ and $p = -1$, respectively.	240
8.52	Temporal profiles of the attachment rate as a function of the magnetic field amplitude and phase difference between the fields for the modified attachment model of Ness and Robson when the attachment cross section is directly proportional to the electron velocity ($p = 0.5$) (black line: $B_0/n_0 = 0$ Hx; red line: $B_0/n_0 = 100$ Hx; green line: $B_0/n_0 = 200$ Hx; blue line: $B_0/n_0 = 500$ Hx; pink line: $B_0/n_0 = 1000$ Hx).	241

8.53	Temporal profiles of the attachment rate as a function of the magnetic field amplitude and phase difference between the fields for the modified attachment model of Ness and Robson when the attachment cross section is inversely proportional to the electron energy ($p = -1$) (black line: $B_0/n_0 = 0$ Hx; red line: $B_0/n_0 = 100$ Hx; green line: $B_0/n_0 = 200$ Hx; blue line: $B_0/n_0 = 500$ Hx; pink line: $B_0/n_0 = 1000$ Hx).	242
8.54	Temporal variation of the bulk and flux longitudinal drift velocity component as a function of the magnetic field amplitude and phase difference between the fields for the modified attachment model of Ness and Robson. The solid, dashed and dotted lines (black line: $B_0/n_0 = 0$ Hx; red line: $B_0/n_0 = 100$ Hx; green line: $B_0/n_0 = 200$ Hx; blue line: $B_0/n_0 = 500$ Hx; pink line: $B_0/n_0 = 1000$ Hx) represent the flux W_z -temporal profiles, the bulk W_z -temporal profiles for $p = 0.5$ and the bulk W_z -temporal profiles for $p = -1$, respectively.	243
8.55	Temporal variation of the flux longitudinal diffusion coefficient $n_0 D_{zz}$ as a function of the magnetic field amplitude and phase difference between the fields for the modified attachment model of Ness and Robson for the same conditions as those in figure 8.51.	244
8.56	Temporal variation of the bulk and flux transverse diffusion coefficient $n_0 D_{xx}$ as a function of the magnetic field amplitude and phase difference between the fields for the modified attachment model of Ness and Robson. The solid and dashed lines (black line: $B_0/n_0 = 0$ Hx; red line: $B_0/n_0 = 100$ Hx; green line: $B_0/n_0 = 200$ Hx; blue line: $B_0/n_0 = 500$ Hx; pink line: $B_0/n_0 = 1000$ Hx) represent the flux profiles and the bulk profiles for $p = -1$, respectively.	244
8.57	Temporal variation of the bulk and flux transverse diffusion coefficient $n_0 D_{yy}$ as a function of the magnetic field amplitude and phase difference between the fields for the modified attachment model of Ness and Robson. The solid and dashed lines (black line: $B_0/n_0 = 0$ Hx; red line: $B_0/n_0 = 100$ Hx; green line: $B_0/n_0 = 200$ Hx; blue line: $B_0/n_0 = 500$ Hx; pink line: $B_0/n_0 = 1000$ Hx) represent the flux profiles and the bulk profiles for $p = 0.5$, respectively.	245
8.58	Schematic diagrams of power absorption in the plasma: (a) no phase difference between the current density and electric field; (b) the phase difference of $2\pi/5$ between the current density and electric field.	247
8.59	The variation of the cycle-averaged mean energy with B_0/n_0 for the Reid ramp model for various (a) field frequencies and (b) phase differences between the fields.	248
8.60	The variation of the temporal profiles of the longitudinal drift velocity component with B_0/n_0 for the Reid ramp model. The electric and magnetic fields are $\pi/2$ out of phase.	249

8.61	The variation of the temporal profiles of the cycle-averaged mean energy with B_0/n_0 for CF_4 . The electric and magnetic fields are $\pi/2$ out of phase.	250
8.62	The 3-dimensional plots of the percentage difference between the two-term and multi-term solution of the Boltzmann equation in $n_0 D_{xx}$ as a function of the phase difference θ between the fields for two applied electric field amplitudes of 12 and 24 Td for the Reid ramp model.	251
8.63	The 3-dimensional plots of the percentage difference between the two-term and multi-term solution of the Boltzmann equation in $n_0 D_{yy}$ as a function of the phase difference θ between the fields for two applied electric field amplitudes of 12 and 24 Td for the Reid ramp model.	251
8.64	The 3-dimensional plots of the percentage difference between the two-term and multi-term solution of the Boltzmann equation in $n_0 D_{zz}$ as a function of the phase difference θ between the fields for two applied electric field amplitudes of 12 and 24 Td for the Reid ramp model.	252
8.65	Comparison between the temporal profiles of $n_0 D_{xx}$ obtained by the two-term approximation (dashed lines) and multi-term theory (full lines). Temporal profiles are given as a function of B_0/n_0 (black line: 0 Hx; red line: 100 Hx; green line: 200 Hx; blue line: 500 Hx; pink line: 1000 Hx) and field frequencies ((a) 10 MHz; (b) 20 MHz; (c) 100 MHz; (d) 200 MHz).	253
8.66	Comparison between the temporal profiles of $n_0 D_{yy}$ obtained by the two-term approximation (dashed lines) and multi-term theory (full lines) for the same conditions as in Fig. 8.64.	254
8.67	Comparison between the temporal profiles of $n_0 D_{zz}$ obtained by the two-term approximation (dashed lines) and multi-term theory (full lines) for the same conditions as in Fig. 8.64.	254
9.1	Spatial relaxation of the mean energy for the step model for a range of reduced electric fields.	257
9.2	Spatial relaxation of the average velocity for the step model for a range of reduced electric fields.	257
9.3	Spatial relaxation of the mean energy for the step model at E/n_0 of 6 Td for different magnitudes of the cross section for elastic collisions.	258
9.4	Spatial relaxation of the mean energy for the step model at E/n_0 of 25 Td starting from the beam initial velocity distribution function with the average electron energies of 0.5, 5, 10 and 20 eV.	260
9.5	Spatial relaxation of the (a) mean energy, (b) average velocity and (c) ionization rate coefficient for the ionization model of Lucas and Saelee at $E/n_0 = 10$ Td. The initial electron energy is 1.5 eV.	260

9.6	Spatial relaxation of the (a) mean energy, (b) average velocity and (c) ionization rate coefficient for modified attachment model of Ness and Robson at $E/n_0 = 10$ Td. The initial electron energy is 1.5 eV.	263
9.7	Spatial relaxation of the mean energy for electrons in argon for a range of reduced electric fields.	265
9.8	Spatial relaxation of the average velocity for electrons in argon for a range of reduced electric fields.	265
9.9	Spatial relaxation of the mean energy (a) and average velocity for electrons in CF_4 for a range of reduced electric fields.	266
9.10	Spatial relaxation of the mean energy for electrons in argon- CF_4 mixture.	267
9.11	Spatial relaxation of the mean energy (first row) and average velocities v_z (second row) and v_x (third row) for the step model at $E/n_0 = 6$ Td for a range of magnetic fields: $B/n_0 = 0$ (first column), 100 Hx (second column), 500 Hx (third column), and 1000 Hx (fourth column).	268
9.12	Spatial relaxation of the rate coefficients for elastic (first row) and inelastic (second row) collisions for the step model at $E/n_0 = 6$ Td for various magnetic field strengths: $B/n_0 = 0$ (first column), 100 Hx (second column), 500 Hx (third column), and 1000 Hx (fourth column).	270
9.13	Spatial relaxation of the mean energy (first row) and rate coefficients for elastic (second row) and inelastic (third row) collisions for the step model at $E/n_0 = 6$ Td for various field orientations: $\psi = 0^\circ$ (first column), $\psi = 30^\circ$ (second column), $\psi = 60^\circ$ (third column), and $\psi = 90^\circ$ (fourth column).	271
9.14	Spatial relaxation of the average velocity components: v_x (first row), v_y (second row) and v_z (third row) for the step model at $E/n_0 = 6$ Td for various field orientations: $\psi = 0^\circ$ (first column), $\psi = 30^\circ$ (second column), $\psi = 60^\circ$ (third column), and $\psi = 90^\circ$ (fourth column).	272
9.15	Spatial relaxation of the average velocity components: v_z (first column) and v_x (second column) for the conservative Lucas-Saelee ionization model ($F = 0$) as a function of B/n_0	273
9.16	Spatial relaxation of the mean energy, z -components of the average velocity and ionization rate as a function of B/n_0 for the Lucas-Saelee ionization model.	273
9.17	Spatial relaxation of the mean energy as a function of the angle between the fields for the Lucas-Saelee ionization model.	274
9.18	Spatial relaxation of the average velocity component along the z -direction as a function of the angle between the fields for the Lucas-Saelee ionization model.	274

9.19	Spatial relaxation of the ionization rate as a function of the angle between the fields for the Lucas-Saelee ionization model.	275
9.20	Spatial profile of the number of electrons as a function of the angle between the fields for the Lucas-Saelee ionization model.	276
9.21	Spatial relaxation of the mean energy (a) and z -component of the average velocity (b) as a function of B/n_0 for the modified attachment model of Ness and Robson.	277
9.22	Spatial profile of the number of electrons as a function of B/n_0 (a) and ψ (b) for the modified attachment model of Ness and Robson.	277

List of Tables

2.1	Cartesian components of the gradient tensor operator.	47
6.1	A comparison of the transport properties for the Reid ramp model as a function of ψ at E/n_0 of 12 Td and B/n_0 of 50 Hx (a) and 200 Hx (b) using the Monte Carlo code (MC) and multi-term code for solving Boltzmann equation (BE). Δ represents the percentage deviation between these two sets of the results.	117
7.1	Comparison between the two-term (TTA) and multi-term (MT) Boltzmann calculations of the diagonal elements of the diffusion tensor as a function of ψ at E/n_0 of 12 Td and B/n_0 of 100 Hx (a) and 1000 Hx (b). Δ represents the percentage deviation between these two sets of the results.	160
9.1	Comparison between the SST and mean energies, as well as accuracy of the low-order truncations of the density gradient expansion for the ionization model of Lucas and Saelee.	261
9.2	Comparison between the SST and flux drift velocities, as well as accuracy of the low-order truncations of the density gradient expansion for the ionization model of Lucas and Saelee.	262
9.3	Comparison between the SST and mean energies, as well as accuracy of the low-order truncations of the density gradient expansion for the modified attachment model of Ness and Robson.	264
9.4	Comparison between the SST and flux drift velocities, as well as accuracy of the low-order truncations of the density gradient expansion for the ionization model of Lucas and Saelee.	264
A.1	A comparison of the mean energy and drift velocity components for the ionization model of Lucas and Saelee as a function of ψ at E/n_0 of 30 Td and B/n_0 of 100 Hx using the Monte Carlo code (MC) and multi-term code for solving Boltzmann equation (BE). Δ represents the percentage deviation between these two sets of the results.	282

A.2	A comparison of the diagonal diffusion tensor elements for the ionization model of Lucas and Saelee as a function of ψ at E/n_0 of 30 Td and B/n_0 of 100 Hx using the Monte Carlo code (MC) and multi-term code for solving Boltzmann equation (BE). Δ represents the percentage deviation between these two sets of the results.	283
A.3	A comparison of the mean energy and drift velocity components for the ionization model of Lucas and Saelee as a function of ψ at E/n_0 of 30 Td and B/n_0 of 200 Hx using the Monte Carlo code (MC) and multi-term code for solving Boltzmann equation (BE). Δ represents the percentage deviation between these two sets of the results.	284
A.4	A comparison of the diagonal diffusion tensor elements for the ionization model of Lucas and Saelee as a function of ψ at E/n_0 of 30 Td and B/n_0 of 200 Hx using the Monte Carlo code (MC) and multi-term code for solving Boltzmann equation (BE). Δ represents the percentage deviation between these two sets of the results.	285
A.5	A comparison of the mean energy and drift velocity components for the ionization model of Lucas and Saelee as a function of ψ at E/n_0 of 30 Td and B/n_0 of 500 Hx using the Monte Carlo code (MC) and multi-term code for solving Boltzmann equation (BE). Δ represents the percentage deviation between these two sets of the results.	286
A.6	A comparison of the diagonal diffusion tensor elements for the ionization model of Lucas and Saelee as a function of ψ at E/n_0 of 30 Td and B/n_0 of 500 Hx using the Monte Carlo code (MC) and multi-term code for solving Boltzmann equation (BE). Δ represents the percentage deviation between these two sets of the results.	287
B.1	A comparison of the mean energy and drift velocity components for the modified attachment model of Ness and Robson as a function of ψ at E/n_0 of 10 Td and B/n_0 of (a) 100 Hx; (b) 200 Hx and (c) 500 Hx using the Monte Carlo code (MC) and multi term code for solving Boltzmann equation (BE). Δ represents the percentage deviation between these two sets of the results.	289
B.2	A comparison of the diagonal diffusion tensor elements for the modified attachment model of Ness and Robson as a function of ψ at E/n_0 of 10 Td and B/n_0 of 100 Hx using the Monte Carlo code (MC) and multi term code for solving Boltzmann equation (BE). Δ represents the percentage deviation between these two sets of the results.	290