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Numerical Simulation of Plasma and Reacting Flows

DISSERTATION

Presented in Partial Fulfillment of the Requirements for
the Degree Doctor of Philosophy in the
Graduate School of The Ohio State University

By

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* * * * *

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ABSTRACT

Plasma and non-equilibrium reacting flows occur in a variety of applications ranging from materials processing to space propulsion. This research models and simulates these plasma and reacting systems, *from first principles using High-Performance Simulation (HPS) techniques.*

Unlike conventional flows, these are characterized by highly varying transport properties, chemical compositions, and are influenced by electric and magnetic fields. A realistic description of non-equilibrium plasmas requires a self-consistent solution of the Boltzmann equation for the electrons with chemical kinetics, flow and electromagnetics. This work is the **first** to address plasma flows coupling the equations describing the flow, chemical and state-specific vibrational kinetics and electromagnetics self-consistently in 2-D axisymmetric geometries. This work lays the foundation for incorporating the Boltzmann equation in flowing plasmas. The compressible Navier-Stokes equations describing the plasma flow is self-consistently coupled with chemical kinetics and electromagnetics in a 2-D axisymmetric formulation. The unsteady governing equations are time-marched to steady-state using the Linearized Block Implicit (LBI) scheme of Briley and McDonald. This model is used to investigate flows in a plasma welding torch and arcjet thrusters.

Of significance is the fact that the models developed herein contain no adjustable parameters and therefore enable direct comparison with experiments. Comparisons of

model predictions with experimental measurements obtained at Phillips Laboratory (Edwards Air Force Base), Stanford University and OSU's Welding Engineering Department show excellent agreement. *This study is the first such detailed description of reacting plasma flows and thus extends the state-of-the-art.* Substantial insight into the underlying physics of reacting and plasma flows has been gained as a result of this work.

This work lays the foundation of realistically modeling molecular plasmas under non-equilibrium conditions. Such models not only provide a better understanding, and hence optimization of existing processes but also empower one to implement on-line process control strategies in manufacturing processes. This can impact design of next-generation processes and chemical deposition reactors, and enable process and quality control.

To my Parents

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CHAPTER 1

INTRODUCTION

The term 'plasma' was coined by Langmuir and Tonks to describe what has been called by some as the fourth state of matter [1]. Plasma is an ionized state of matter in solid, liquid or gaseous form, electrically neutral on length scales much larger than the Debye length. The gaseous form is one that is extensively studied. The basic difference between a neutral gas and a plasma arises due to the character of the inter-particle forces. Unlike the gaseous form wherein the force is the weak short-range Van der Waals' type, the collective motion of particles in a plasma are largely dictated by long-range Coulomb interactions. Thus, a plasma is a collection of charged particles, overall electrically neutral on a macroscopic scale, influenced by Coulomb interactions between electrons and ions and by the presence of magnetic fields, either applied externally or self-generated by current flows within the plasma.

Plasmas encompass a variety of distinguishable length scales, ranging from atomic to the galactic. It is estimated that 99% of the universe is made up of plasmas. Lightning, St. Elmo's fire, the Aurora Borealis, and the ionosphere are examples of naturally occurring terrestrial plasmas. Plasmas can also be created under laboratory conditions. Electrical gas discharges are the most popular methods for producing laboratory plasmas.

1.1 Classification and Characteristics of Plasmas

Low and High Temperature Plasmas

Based on the density of the charged particles present, plasmas can be broadly classified into two categories - low-temperature plasmas which can be weakly or fully ionized, and high-temperature plasmas characterized by high charged particle energies. The density of the charged particles (electrons and ions) in low-temperature gas discharges is usually much lower than the density of neutral particles (atoms and molecules). Hence these are also called weakly ionized plasmas. Since the mean translational energy of the electrons or ions is much lower than the ionization potential of the gas particles - these plasmas are sometimes referred to as low-temperature plasmas ($T < 1-5$ eV). High-temperature plasmas, on the other hand are characterized by high charged particle densities with mean translational energies of the heavy particles being on the order of the ionization potential or higher. Fusion plasmas are the best examples of high-temperature plasmas with heavy particle temperatures $T > 10-100$ eV.

Thermally Non-Equilibrium Plasmas

In high-temperature high pressure plasmas, elastic collisions between the electrons and heavy particles dominate. This establishes a thermal equilibrium between the electrons and heavy particles. In other words, a single temperature can be used to describe the state of the plasma. Low-temperature, low pressure plasmas on the other hand exhibit a departure from thermal equilibrium. This is due to the fewer elastic collisions that the electrons suffer with the heavier particles (ions and neutrals) as compared with themselves. This thermal dis-equilibrium adds an additional level of difficulty in the investigation of these low-temperature plasmas.

Thermal dis-equilibrium in low-temperature plasmas is explained on the basis of the energy transfer mechanism between the electrons and the heavy particles. Electrons pick up energy from the applied electric field due to their low mass. These high energy electrons then exchange energy with the heavy particles via elastic and inelastic collisions. However, only a very small fraction of the electron energy is transferred to the heavy particle in each elastic collision due to the large difference in the masses of the electrons and heavy particles (atoms, molecules, ions etc.). Hence, the elastic energy transfer process is very inefficient. In contrast, an elastic collision between two heavy particles can lead to significant amounts of energy transfer as the masses of the colliding partners are comparable. In low-temperature plasmas wherein the ionization levels are very low, the frequency of collisions between the electrons and heavy species is relatively very low. This low collision frequency often results in a situation where the electrons equilibrate among themselves at a temperature T_e and the heavy particles equilibrate at a temperature T_H with $T_e \gg T_H$. An inelastic collision between an electron and a heavy particle, on the other hand, is very efficient in terms of energy transfer. In fact, simple consideration based on conservation of energy and momentum show that up to 99.9% of the electron energy can be transferred to the heavy colliding partner in an inelastic collision [2].

Inelastic collisions can lead to one of many processes - ionization, dissociation, electronic excitation, vibrational excitation etc. In inelastic collisions, the energy lost by the electron is not used up entirely to increase the translational energy of the

heavy particle. Inelastic collisions can lead to more complex situations of thermal disequilibrium as will be explained later in the discussion on atomic and molecular plasmas. Lack of thermal equilibrium is an important characteristic of low-temperature plasmas which distinguishes it from the high-temperature plasmas.

Atomic Plasmas

Low-temperature, low pressure plasmas can be further divided into atomic and molecular plasmas. Atomic plasmas comprise of electrons, ionized atoms and neutral atoms. Since atoms lack vibrational and rotational degrees of freedom, inelastic collisions can lead only to electronic excitation of the atoms and ions. The unexcited neutral atoms can be described by a Boltzmann distribution at a temperature T_H . If there exists a sufficient number of collisions per unit time between the electronically excited states and the neutral atoms to establish equilibrium between translational and electronic modes, it is possible to describe these electronically excited states also by the heavy particle temperature, T_H . In other words, the heavy particles (neutrals and ions) can be described by a Maxwellian or a near Maxwellian distribution at the temperature T_H . However, if strong coupling between the inelastic processes and the electron energies exist, then the electron energy distribution function (EEDF) may well be non-Maxwellian. If the radiative processes are out of equilibrium, the description of the plasma is more complicated. Under such circumstances, the distribution of the electronically excited states will be non-Maxwellian and hence it is not possible to ascribe a single temperature to describe the atoms and ions. In such cases, the ions and excited neutrals have temperatures distinct from cold neutrals (T_H) so that a three or more temperature description ($T_e, T_H \neq T_i$) is necessary. However, in most cases of interest the heavy particles and the electrons are indeed in equilibrium

amongst themselves respectively. Hence in most practical cases a two-temperature description of plasmas is fairly accurate, where the electrons are characterized by a temperature T_e and the heavy particles are characterized by T_H , with T_e usually much greater than T_H .

Low Pressure Molecular Plasmas

Molecular plasmas comprise of electrons, ionized molecules, ionized atoms, neutral atoms, and neutral molecules. The presence of diatomic or polyatomic molecules in neutral or ionized form complicates matters further. This is due to the fact that diatomics and polyatomics can also store energy in rotational and vibrational modes in addition to electronic excitation. A molecule has a number of discrete electronic levels. With each electronic level is associated a set of vibrational energy levels, and associated with each of these vibrational levels there are a set of rotational levels. A molecule can be in one of these many states.

In an isolated thermodynamic system at equilibrium, the population of molecules in different energy levels is governed by the Boltzmann distribution. Every system that is out of equilibrium eventually relaxes to an equilibrium state as required by the second law of thermodynamics. However, in systems that are not isolated, there may exist non-equilibrium distributions. This is due to the fact that the individual relaxation times of the various internal states of molecules can differ by several orders of magnitude. Relaxation to equilibrium is determined by the relative importance of inelastic collisions. The energy of one colliding particle may be channeled into one of the several internal modes of the collision partner, namely vibration, rotation or electronic excitation. Inelastic collisions involving these internal modes often render them out of equilibrium with the external modes of molecular motion (i.e.

translation). Rotational relaxation rates are typically the fastest, requiring only a few collisions to equilibrate with the translational modes. The number of collisions required to equilibrate the vibrational modes is however, much greater than that required for rotation, on the order of millions of collisions (at pressures on the order of a few torr). The long relaxation times for vibrational modes often lead to situations where the resulting populations of vibrational states are markedly non-Boltzmann. When vibration-vibration (VV) collisional processes dominate vibration-translational (VT) processes the populations of the vibrational states follow the Treanor-Rich distribution [3]. In the range of electronic energies of 0.5-3.0 eV collisions resulting in vibrational and electronic excitation dominate electron-molecule energy exchange processes [4]. The non-Boltzmann distribution of the internal modes tends to make the EEDF non-Maxwellian as well, with the result that a single electron temperature cannot be defined. In such situations, there is no recourse but to calculate the EEDF from the electron-molecule collision rates with electron transport coefficients averaged over the EEDF. Although this is the usual case, there are rare instances (eg. gas mixtures with fast V-T relaxers) when elastic collisions dominate and the two-temperature or at worst, three-temperature description used for atomic plasmas is applicable to molecular plasmas.

The above discussion on the characteristics of plasmas underscores the fact that high-temperature plasmas can often be described by a single temperature while many low-temperature plasmas cannot. The above mentioned characteristics of low-temperature plasmas, namely the importance of inelastic collisions, shows their complex nature. Hence their investigation is fraught with numerous difficulties. However,

these plasmas are important in a host of applications which make it imperative to develop tools to study their nature and characteristics in greater detail.

1.2 Plasma Applications

Plasmas, both high and low-temperature, have many applications. Controlled thermonuclear fusion is the most widely publicized high-temperature plasma application. Low-temperature, low pressure, collision-dominated plasmas have a host of industrial applications such as spraying, coating, welding and materials processing.

Typically, low-temperature collision dominated plasmas have average electron energies in the range of 1-5 eV and pressures between 1 torr and 1 atm. These plasmas have electric fields that can impart significant energy to the electrons and drive chemical reactions while maintaining low heavy particle temperatures. This distinguishing feature of low-temperature plasmas has important applications in the areas of materials modification and processing - fabrication of semiconductors, being one of the most technologically important. Plasma sources that provide positive and negative ions are used to implant ions into materials, deposit thin films or etch miniscule structures. This process is employed in the fabrication of semiconductor circuits. The life and reliability of high-performance engines is increased by the hardening of bearings using techniques such as ion-implantation or coatings. Other important uses of low-temperature plasmas include the "cold" pasteurization of food products, the sterilization of medical products, gas discharges for lighting and lasers, isotope separation, switching and welding technology, environmental cleanup, and space propulsion systems [5].

1.3 Methods of investigating plasmas

Use of plasmas in the aforementioned applications requires the optimization of plasma parameters of interest such as the number densities of the reacting species and discharge electrical characteristics. A basic understanding of electron-impact excitation phenomena, presence of vibrational and electronically excited states, stability of a given discharge configuration, interaction between the plasma and surfaces, electron-impact kinetics, and the EEDF in low-temperature plasmas are of vital importance. These become especially crucial when coupled to a flow field. The plasma medium is inherently nonlinear as the charged particles comprising it interact collectively with self-generated or externally applied electromagnetic fields produced by the charge density and currents associated with the net flux of plasma particles. The study of these systems is further complicated due to their largely non-equilibrium thermodynamic state. More importantly, most low-temperature plasma applications involve complex reactions between electrons and a host of atomic, molecular and ionic species. These ionic species are found in highly excited states, not usually encountered in non-plasma environments.

Experimental and theoretical approaches have sought to delve deeper into the behaviour of these plasmas. However, such complex plasma systems are not easily amenable to experimental probing due to their hostile environments. Limited experimental data on temperatures and species number densities are available for select cases. Recent advances in experimental techniques and instrumentation have made it possible to obtain some information about state-specific kinetics¹.

¹State-specific kinetics refer to the collisional interactions (V-V, V-T, V-E, etc.) between individual molecular energy states, as functions of specific electronic levels, and vibrational and rotational quantum numbers.

As in several other areas of scientific inquiry, theoretical approaches complement experimental efforts directed at gaining a better understanding of plasmas. Theoretical approaches essentially consist of describing physical phenomena in a rationally derived mathematical form (called governing equations), revealing the dominant physical mechanisms with the appropriate initial and boundary conditions. This description is known as a model of the system. For simple physical systems, direct analytical solutions of the governing equations can be obtained using established mathematical techniques. At times, asymptotic solutions can also be obtained. When analytical solutions of models describing a complex system cannot be obtained, one must resort to numerical methods. The technique of using numerical methods to obtain solutions to a model describing a system is known as numerical simulation. Numerical simulation requires a computational representation of the physical system under consideration to be constructed. This is accomplished by choosing and applying relevant computational techniques and approximations. Certain simplifications are made to make the solution tractable, but one has to exercise a great deal of caution to ensure that the relevant physics is retained despite the simplifications.

The complex nature of plasmas belies hopes of obtaining direct analytical solutions for most practical configurations. Numerical simulations of such plasmas promise to provide a framework for interpreting observed experimental data through better understanding of the underlying physical processes. Numerical simulations provide us with information of interest (such as temperature and species concentration), in regions often inaccessible to experimentalists. Developing reliable models for these plasmas holds the key to vastly improving the operation of devices such as plasma reactors and arc-discharges.

A rigorous formulation of problems involving flowing plasmas is a daunting task. However, approximate formulations provide considerable insight into important phenomena. These methods are classified as follows:

1. *Equilibrium theory*
2. *Orbit theory*
3. *Magnetohydrodynamic formulation*

Equilibrium theory rests on the premise that collisions between charged particles lead to the well-known Maxwell-Boltzmann equilibrium distribution of particle velocities in the body of the plasma. Kinetic and transport properties are then calculated from this Maxwell-Boltzmann velocity distribution function. *Orbit theory* treats the motion of charged particles under the influence of electric and magnetic fields. It is a good approximation when collisions are infrequent. The mean free paths are much longer than the orbits of individual particles. Collective motion of the particles in a collision-dominated plasma is best handled by the *magnetohydrodynamic formulation*. According to this description, the plasma is treated as an electrically conducting fluid (thus also influenced by magnetic fields) which also obeys the conventional equations of hydrodynamics. The behavior of such a conducting fluid is complicated by the presence of electromagnetic phenomena. Hence, the classical fluid equations are solved in conjunction with Maxwell's electromagnetic equations. This serves as a good description when the mean free path for collisions is small compared to dimensions of physical interest. The Navier-Stokes equations in conjunction with the overall continuity equation, species continuity equations, energy equation(s) and

Maxwell's equations under the MHD approximations are collectively known as the MHD equations [6].

As pointed out earlier, study of molecular plasmas is greatly complicated under non-equilibrium conditions. In principle, one could construct a computational representation of these molecular plasmas by “simply” solving the time and spatially dependent Boltzmann equation for each species. Consideration of non-equilibrium conditions would require each of the atomic and molecular states of each of the constituents in the plasma to be treated as a distinct specie. This approach would be intractable even for a single specie. A relatively simplified description would however consider all heavy species to be describable by a single bulk gas temperature. A realistic description of the non-equilibrium kinetics requires a self-consistent solution of the Boltzmann equation for the electrons (describing the electron energy distribution function (EEDF)) and the species conservation equations. The source terms in the species equations comprise of terms describing the time rate of change of population of a given specie due to inelastic collisional processes such as Vibration-Translation (V-T), Vibration-Vibration (V-V), Vibrational-Electronic (V-E), and chemical reactions. Since electron-molecule collision rates (which describe the various elastic and inelastic collisions) and the electron transport coefficients are averaged over the distribution of electron energies, evaluation of these quantities requires a knowledge of the EEDF and the factors that influence it. Hence a coupled approach is necessary. An overall energy equation for the fluid describes the evolution of the heavy particle temperature. To describe a flowing plasma an equation describing the evolution of the EEDF has to be coupled with the MHD equations (assuming the flow is collision dominated). This set of equations being coupled, unsteady, and highly non-linear,

does not lend itself to analytical solutions for any but the most simplified cases. There is therefore no recourse but to resort to numerical methods for the solution of these equations.

1.4 Issues in the modeling of plasmas

Numerical simulation of the behavior of plasmas is far from trivial. Some of the crucial issues in the modeling of plasmas are discussed next.

1. A model must be capable of incorporating the effects of phenomena with disparate length and time scales. For example, in a simulation involving reacting flow through a C-D nozzle, one has to contend with convective time-scales and time-scales of reactions or other processes which may differ by many (often tens of) orders of magnitude. Similarly, processes taking place near surfaces or boundary layers do not occur on the same spatial scale as the bulk of the plasma.
2. Time integration of the governing equations describing plasmas is greatly complicated by stiffness. Stiffness in these equations is due to the widely differing time-scales describing the coupling of several physical phenomena. Time marching these stiff equations to steady-state can place stringent demands on the available computational resources. This is due to the fact that the size of the time-step that can be used in the time-marching scheme is dependent on the method of time integration. The two forms of time integration used in finite-difference approaches are the *explicit* and the *implicit* methods. *Explicit* methods express the dependent variable(s) at a given time level entirely in terms of quantities known at the previous time level. In other words, there is only one

unknown in the difference equation, entirely expressed in terms of known quantities. *Implicit* methods, on the other hand, are computationally more involved. The reason being that more than one unknown appears in the difference equation at a given time level, thus requiring the simultaneous solution of several non-linear equations involving the unknowns. The choice of approach, namely, *Explicit* or *Implicit* is dictated by the time-scales that need to be resolved, the relation of the time-steps to the stability limits of the particular algorithm used, and the stiffness of the governing equations. The size of the time-step used in these computations is dictated by the need to resolve the fastest process important to the system. In reacting plasma flows, convective time-scales may differ from the time-scales describing reactions by as much as thirty to forty orders of magnitude. Due to this large disparity in time-scales, these problems are best handled by implicit methods of time integration. This means that a considerable amount of effort has to be expended in code development. Use of explicit methods would either make the time needed for computations impractical or in some cases lead to numerical instability. This is one of the main reasons why *there does not presently exist a detailed plasma flow model describing the coupling between convection, chemical kinetics, electromagnetics and the inclusion of a self-consistently evaluated EEDF.*

3. The effects of numerical diffusion, dispersion, and aliasing errors [7, 8] are more acute in the numerical solution of reacting plasma flows. Governing equations describing plasma flows include several phenomena which make the numerical solution of these problems more involved when compared to problems involving ordinary flows. The effects of numerical artifacts (diffusion and aliasing) in such

complex problems are not well understood. New and efficient algorithms which minimize these numerical effects are needed.

4. Benchmarking numerical simulations with analytically derived asymptotic results (when available) or with experimental results is of utmost importance. This is especially so when numerical models employ the full set of equations describing the processes occurring in the plasma. This allows assessment of the accuracy and resolution of the numerical solution. Further, it allows discrimination of physically viable results from those that are mere numerical artifacts. Validation of results of numerical solutions against experimental data is however, beset with problems. Non-conformity of experimental and numerical solutions could be not only due to numerical artifacts but also due to a lack of knowledge of fundamental properties describing the system. Knowledge of transport properties (viscosity, thermal conductivity, electrical conductivity, species diffusivities and mobilities) and their variations, rate constants and cross-sections for various reactions are all of great importance. Transport properties provide the vital link between microscopic processes and the macroscopic flow characteristics. Only a limited amount of experimental data are available for these transport properties and virtually none under non-equilibrium conditions. These properties are tensorial quantities and their precise evaluation requires the evaluation of the non-equilibrium velocity distribution function. Transport properties evaluated using the simpler mean-free-path theory can be in error by a factor of two or three [9]. Rate constants and cross-sections for the myriad processes taking place in reacting plasmas are also not always known.

Experimentally determined rates and cross-sections are known for some processes. However, these values are known over limited temperature and pressure ranges that may not span the entire range of interest covered in a numerical simulation. Moreover, the rates can be in error by as much as an order of magnitude. These uncertainties in rates and properties can affect the results of simulations and lead to apparent disagreement with experiments, while the physics might be captured correctly. Models are incapable of including effects of plasma-surface interactions and gas purity. Effects of deterioration of surfaces can lead to considerable scatter in experimental results. This uncertainty can also cause disagreement between predicted results and experimental measurements. Finally, constraints or boundary conditions specified in a model may not be the same as those in an experiment. This makes it very important for comparison between experiment and model to be based on the same “platform”.

5. Computational resources in terms of storage and clock-speed are necessary for advancement of the state-of-the-art of numerical simulations of plasma flows. Realistic description of reacting plasma flows requires the inclusion of state-specific kinetics and plasma chemistry. Inclusion of these effects increases the number of coupled equations by a considerable amount. Highly efficient algorithms and advanced computer systems are thus required to obtain steady-state solutions to these large systems of equations in a reasonable amount of time.

1.5 Background

Until recently, lack of computing resources greatly hindered progress in the area of numerical computation of plasma flows, largely due to the stiffness of the governing

equations. Moreover, results of numerical simulations of plasma flows could not be benchmarked due to non-availability of reliable experimental data. Despite these hinderances, efforts have been on-going to develop computational tools and techniques aimed at examining different aspects of flowing plasmas.

A great deal of work on investigation of coupled phenomena involving stiff equations exists. Oran and Boris [7] address numerical solution of stiff equations and give a fairly exhaustive review of existing work in the area. The earliest efforts in solving coupled equations with stiffness were directed toward rate equations describing chemical reactions [7]. These equations were however not coupled to the flow field. Also, a plethora of investigations exist on numerical solutions of the Navier-Stokes equations. These studies examine 2-D and 3-D Navier-Stokes equations for viscous and inviscid, supersonic and subsonic, internal and external flows[7, 10].

Efforts have also been made to combine flow fields with finite-rate chemical kinetics. Oran and Boris [7] discuss attempts to combine convection and detailed chemical kinetics for solving flows with shocks and detonations in 1-D. They however point out that multi-dimensional, time-dependent, compressible codes such as FAST2D, and FAST3D, are unable to include detailed chemical kinetics as in the 1-D case. This is primarily due to the enormous computational resources required.

In comparison to reacting flows, *reacting plasma flows* involve an additional degree of complexity. This is due the fact that these flows require coupling between the flow field, chemical kinetics and electromagnetics. As explained earlier, modeling of chemical kinetics in molecular plasmas is computationally very intensive if one considers state-specific kinetics. Various groups around the world have attempted to model atomic and molecular plasmas, in electric discharges [11]. Realistic models

describing these kinds of discharges need comprehensive models coupling the above mentioned effects. A large body of literature addresses the coupling between the EEDF and master equations describing molecular energy transfer [11]. Most of these studies do not include the effects of plasma chemistry. Further, these studies do not include the effects of electromagnetics or convection, and are therefore limited in their usefulness for real engineering applications.

Recent attempts to model flows in arcjet thrusters have led to several investigations of reacting flows including electromagnetics effects. Chapter V gives details of studies performed by coupling the flow equations with electromagnetics. However, none of these investigations address state-specific kinetics. Attempts have been made to include state-specific kinetics along with convection in 1-D flows [12, 13]. These attempts did not however include the effects of electromagnetics. Also in these studies, no attempt is made to couple the flow field and chemical kinetics with the EEDF (a necessity for molecular plasmas) and a single temperature is assumed to represent the gas.

As pointed out earlier, there exist no studies to-date that include state-specific chemical kinetics, flow, and electromagnetics, coupled self-consistently with the EEDF which can realistically describe reacting molecular plasma flows.

1.6 Motivation for the present work

Problems related to plasma flows are excellent examples of complex physical phenomena, coupling many interactions. Lack of a comprehensive model describing the four major interactions, namely flow, electromagnetics, state-specific chemical kinetics and the effects of the EEDF, is the single most important motivation for the

present work. Availability of experimental data and computing resources is another. Solutions to large sets of governing equations encountered in plasma flow simulations are possible in reasonable amounts of time due to advances in high-speed computing. Furthermore, the past few decades have produced a great deal of information regarding rate coefficients describing chemical reactions including those originating in specific states and terminating in others. Modern experimental techniques and instrumentation to interrogate atomic and molecular plasmas are largely responsible for this advancement.

Investigating molecular plasmas under non-equilibrium conditions promises not only to better understand and optimize existing processes but also empower one to implement on-line process control strategies in manufacturing processes. *An all-encompassing numerical model capable of addressing all the above-mentioned interactions would significantly improve the understanding of low-temperature plasma flows.* This can impact design of next-generation processes and chemical vapor deposition reactors, and enable better process and quality control.

1.7 Goals of this work

The unprecedented increase in computing resources (in terms of clock speed and memory) in recent years has spurred a great deal of interest in the use of computational methods in science and engineering. Computational approaches have the potential advantage of cost-effectiveness over experimental techniques especially in design and scale-up. High-performance simulation methods promise to enable solutions to complex systems of equations in reasonable amounts of time. High-performance simulations aim to develop algorithms and codes designed to exploit the architecture

and memory configuration of modern computers to the fullest extent. A touchstone used to gauge the performance of a code is the number of million floating point operations per second or Mflops (for Mega-flops). It is absolutely essential to structure codes astutely in order to extract maximum performance on a given computer, so as to produce results in the shortest possible amount of time.

The goal of this dissertation is to develop and apply high-performance simulations to multidimensional plasma and reacting flows (internal and external) and utilize the insight gained from these simulations to explore the behavior of non-equilibrium low-temperature, plasma flows.

The present work uses the computational resources at our behest and the availability of experimental data describing various inelastic processes between electrons and molecules (N_2 , CO , etc.) to study and explore reacting plasma flows. Obtaining a realistic description of non-equilibrium plasma flows requires a self-consistent solution of the Boltzmann equation for the electron energies together with the chemical kinetics, flow and electromagnetics. *This study is the first such detailed description of reacting plasma flows and thus extends the state-of-the-art.* Substantial insight into the underlying physics of such flows has been gained as a result of this work.

Fluid description of plasmas, self-consistently coupled with chemical kinetics and electromagnetics in a 2-D axisymmetric formulation is used. The governing equations describing these flows are time-marched to steady-state. The Linearized Block Implicit (LBI) scheme of Briley and McDonald [14] is used. Chapter III discusses the reasons for the selection of this technique in the present work. Although the LBI algorithm was initially developed to solve the compressible Navier-Stokes equations in multi-dimensions, the present work is the first to extend this scheme to study

reacting molecular plasma flows. A variety of flows through different geometrical configurations have been studied in order to demonstrate the wide applicability of the LBI method. Although no turbulence effects are included in the case studies presented in this dissertation, the numerical algorithm can easily accomodate them, given a suitable turbulence model, or directly as in DNS (Direct Numerical Solutions of Navier-Stokes Equations) simulations.

The low-temperature plasmas under consideration have regions of slow and fast flows, as well as regions of high and low pressures. Developing a modular code capable of handling these different regimes of flow coupled with chemical kinetics, diffusive transport and electromagnetic effects without sacrificing computational performance has been accomplished in this work. This work lays the foundation for solution of the Boltzmann equation for electron energies unified with the fluid description of plasmas. To the best of this author's knowledge there exist no similar simulations currently capable of handling the complexity of low-temperature plasma flows in terms of generality, speed and accuracy. Development of such an all-encompassing high-performance modular code has greatly extended the state-of-the-art in the study of plasma discharges. The ability of the LBI scheme to time-march accurately in a stable manner will enable its use as a design tool and eventually for on-line process control. In addition, the tools developed in this dissertation may be used to study myriad problems of fundamental interest in plasma physics.

This dissertation is organised as follows. The governing equations and problem formulation are discussed in chapter II. The LBI method and its extention to plasma flows are discussed in chapter III. Code verification is addressed in Chapter IV. Chapter V and VI form the core of this work. Case studies specific to plasma propulsion

and plasma welding are discussed in chapter V. Chapter VI describes a solution technique to include the EEDF with electromagnetics and flow. It also discusses the coupling of state-specific vibrational kinetics with flow in 2-D axisymmetric nozzles with large area ratios. This is a necessary first step in the incorporation of the Boltzmann equation for the EEDF to describe molecular plasmas. Finally, Chapter VII gives a brief summary of this research and concludes with recommendations for future research.

CHAPTER 2

GOVERNING EQUATIONS AND FORMULATION

Formulation of a problem involves describing the governing equations along with the boundary and initial conditions. It also involves the description of other physical quantities (such as properties) which characterize a system. In deriving the governing equations a number of simplifying assumptions are made. For present purposes, a continuum description is assumed to hold good which allows the plasma to be treated as a conducting fluid. This approximation is valid in the reacting plasma flows studied in this work since the particle densities are high. The continuum approximation allows the macroscopic conservation of mass, momentum and energy to describe the flowing plasma system.

The basic equations that govern flowing plasmas (under the continuum approximation) are essentially the compressible Navier-Stokes equations. These plasmas are typically composed of electrons, ions, neutral atoms and molecules, ions and molecular ions. A complete description of these flowing plasmas requires the flow equations to be coupled with an energy equation (or several energy equations), species continuity equations and Maxwell's equations. The solution of this set of equations is indeed a daunting task. Variable properties, presence of $\vec{j} \times \vec{B}$ body forces, Ohmic heating,

species diffusion, chemical reactions with ionization/recombination, rotational, vibrational and electronic mode non-equilibrium make these system of equations extremely non-linear and stiff, making them very difficult to solve.

This chapter discusses the formulation of problems concerning plasma flows. We begin by describing the vector form of the governing equations first. These general equations are then rewritten in cylindrical coordinates assuming axisymmetry. The 2-D form of these equations is then applied to the geometric configurations for the case studies in this work. This is followed by a discussion on non-dimensionalization of these equations. Transport properties essential to the description of these plasmas are discussed next. This chapter is finally concluded with a discussion of certain general initial and boundary conditions used in modeling plasma flows.

2.1 Vector Forms of the Governing Equations

Vector equations in conservative form describing non-equilibrium plasmas are described in this section [6, 15]. Equation 2.1 describes the continuity equation.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \quad (2.1)$$

$$\frac{\partial}{\partial t} (\rho \vec{v}) + \nabla \cdot \rho \vec{v} \vec{v} = -\nabla p + \vec{F} - \nabla \times [\eta (\nabla \times \vec{v})] + \nabla \left[\frac{4}{3} \eta \nabla \cdot \vec{v} \right] \quad (2.2)$$

Equation 2.2 describes the momentum equations. Equations describing the conservation of momentum are also known as the Navier-Stokes equations. $\vec{F}$ on the right hand side of equation 2.2 denotes the net body force per unit volume. These equations must be supplemented by an equation for conservation of energy for each species.

$$\frac{\partial}{\partial t} e_{T_i} + \nabla \cdot ([e_{T_i} + p_i] \vec{v}) = -\nabla \cdot \vec{q} - \nabla \cdot \vec{q}_r + \dot{q}''' + \eta \Phi + \sum_j \Delta E_{ij} \quad (2.3)$$

The above form of the energy equation can be applied to a species i with a translational temperature T_i . The term $-\nabla \cdot \vec{q}$ on the right hand side of equation (2.3) is the net energy per unit volume transferred by heat conduction and diffusion, $-\nabla \cdot \vec{q}_r$ is the net energy per unit volume transferred by radiation, and q''' is the energy generated per unit time per unit volume. For a conducting fluid, $q''' = \vec{j} \cdot \vec{E}$ under the MHD approximation [6], and $\mu\Phi = \vec{v} \cdot \nabla \cdot \vec{\tau}$ is the the rate at which work is done by surface forces. $\sum_j \Delta E_{ij}$ represents the energy exchange per unit volume between the species i and species j . In the above energy equation, each specie i is assumed to be characterized by a translational temperature T_i . This inherently assumes that the velocity distribution function is locally given by the Maxwell-Boltzmann distribution. As pointed out in chapter I, in a two temperature description of a plasma comprising of heavy particles and electrons, all the heavy particles are assumed to be characterized by a single temperature T_h and the electrons are characterized by a temperature T_e . In such a situation, T_i in the various energy equations would be replaced by a single temperature T_h to yield an energy equation for the heavy particles. A similiar equation is then written for the electrons.

In addition to the equations governing the conservation of mass, momentum and energy, it is necessary to describe the time-evolution of the various species in the plasma. Species in a plasma may be monatomic or polyatomic. The monatomic species have only one internal mode - that of electronic excitation. Polyatomic species on the other hand have states of rotation and vibrational in addition to electronic excitation. Each of these different internal states can be treated as a specie with a separate equation governing its evolution. The species equations for monatomic and polyatomic species are described below:

$$\frac{\partial n_m}{\partial t} + \nabla \cdot (n_m \vec{v}) + \nabla \cdot \left(-n_m \mu_m \vec{E}' + \frac{D_m}{k_b T_m} \nabla \cdot (n_m k_b T_m) \right) = n_m \quad (2.4)$$

$$\begin{aligned} \frac{\partial n_{iv}}{\partial t} + \nabla \cdot (n_{iv} \vec{v}) + \nabla \cdot \left(-n_{in} \mu_{iv} \vec{E}' + \frac{D_{iv}}{k_b T_{iv}} \nabla \cdot (n_{iv} k_b T_{iv}) \right) \\ = VT_{i,v} + VV_{i,v} + SRD_{i,v} + n_{i,v} \end{aligned} \quad (2.5)$$

2.2 Governing Equations in 2-D Axisymmetric Form

For our present purposes, we consider the governing equations in cylindrical polar coordinates in 2-D axisymmetric form. A single temperature is used to describe all the components of the plasma, so that there is only one energy equation. The continuity equation, radial, axial and azimuthal components of the momentum equations, the energy equation and the species (monatomic and diatomic) equations, are discussed next in dimensional, conservative form.

Conservation of mass is expressed by the continuity equation:

$$\frac{\partial \rho^*}{\partial t^*} + \frac{1}{r^*} \frac{\partial}{\partial r^*} (r^* \rho^* u^*) + \frac{\partial}{\partial x^*} (\rho^* w^*) = 0 \quad (2.6)$$

where, the asterisks denote dimensional quantities.

Conservation of momentum in the radial, azimuthal and axial directions are:

$$\begin{aligned} \frac{\partial}{\partial t^*} (\rho^* u^*) + \frac{1}{r^*} \frac{\partial}{\partial r^*} (r^* \rho^* u^{*2}) + \frac{\partial}{\partial x^*} (\rho^* u^* w^*) - \frac{\rho^* v^{*2}}{r^*} \\ = -\frac{\partial p^*}{\partial r^*} + \frac{\partial}{\partial r^*} \left[2\eta^* \frac{\partial u^*}{\partial r^*} - \frac{2}{3} \eta^* \nabla \cdot \vec{u}^* \right] - j_x^* B_\theta^* \\ + \frac{\partial}{\partial x^*} \left[\eta^* \left(\frac{\partial u^*}{\partial x^*} + \frac{\partial w^*}{\partial r^*} \right) \right] + \frac{2\eta^*}{r^*} \left(\frac{\partial u^*}{\partial r^*} - \frac{u^*}{r^*} \right) \end{aligned} \quad (2.7)$$

$$\frac{\partial}{\partial t^*} (\rho^* v^*) + \frac{1}{r^*} \frac{\partial}{\partial r^*} (r^* \rho^* u^* v^*) + \frac{\partial}{\partial x^*} (\rho^* v^* w^*) - \frac{\rho^* u^* v^*}{r^*}$$

$$\begin{aligned}
&= \frac{\partial}{\partial r^*} \left[\left(\eta^* \frac{\partial v^*}{\partial r^*} - \frac{v^*}{r^*} \right) \right] + \frac{\partial}{\partial x^*} \left[\eta^* \frac{\partial u^*}{\partial x^*} \right] \\
&\quad + \frac{2\eta^*}{r^*} \left(\frac{\partial v^*}{\partial r^*} - \frac{v^*}{r^*} \right)
\end{aligned} \tag{2.8}$$

$$\begin{aligned}
&\frac{\partial}{\partial t^*} (\rho^* w^*) + \frac{1}{r^*} \frac{\partial}{\partial r^*} (r^* \rho^* u^* w^*) + \frac{\partial}{\partial x^*} (\rho^* w^{*2}) \\
&= -\frac{\partial p^*}{\partial x^*} + \frac{\partial}{\partial x^*} \left[2\eta^* \frac{\partial w^*}{\partial x^*} - \frac{2}{3} \eta^* \nabla \cdot \vec{u}^* \right] - j_r^* B_\theta^* \\
&\quad + \frac{1}{r^*} \frac{\partial}{\partial r^*} \left[\eta^* r^* \left(\frac{\partial u^*}{\partial x^*} + \frac{\partial w^*}{\partial r^*} \right) \right]
\end{aligned} \tag{2.9}$$

In the above equation, u, v and w are the radial, azimuthal and axial components of velocity, respectively. It must be pointed out that in the above equations, the bulk viscosity is assumed to be zero. This is true for dense gases. It is identically zero for low density monatomic gases [15]. The bulk viscosity is a measure of energy transfer from the translational modes to the other internal modes [16]. In this work, a single temperature is assumed to characterize all the particles. In other words, the translational modes are assumed to be in equilibrium with the other internal modes. For the cases studied in this work, this assumption is valid since the operating pressures (200 - 200,000 Pascals) are high, ensuring a high collision frequency. However, the bulk viscosity is important in problems involving acoustic or shock-waves, since this produces viscous decay of the high-frequency waves [15].

The energy equation can be written as:

$$\begin{aligned}
&\frac{\partial e_T^*}{\partial t^*} + \frac{1}{r^*} \frac{\partial}{\partial r^*} ([e_T^* + p^*] u^* r^*) + \frac{\partial}{\partial x^*} ([e_T^* + p^*] w^*) \\
&= \frac{1}{r^*} \frac{\partial}{\partial r^*} \left(k^* r^* \frac{\partial T^*}{\partial r^*} \right) + \frac{\partial}{\partial x^*} \left(k^* \frac{\partial T^*}{\partial x^*} \right) \\
&\quad + \eta^* \Phi^* + j_r^* w^* B_\theta^* - j_x^* u^* B_\theta^* + \frac{j_r^{*2} + j_x^{*2}}{\sigma}
\end{aligned} \tag{2.10}$$

The energy equation is written describing the transport of total energy, i.e. internal energy + kinetic energy, under the assumption of a single temperature (i.e. the electrons are assumed to have the same mean thermal energy as the heavy particles or the ions). This is not strictly true as the electrons lose only a fraction of their energy per elastic collision. A two-temperature model would entail solving another equation governing the energy conservation for the electrons. The aforementioned equation would then resemble the conservation equation for electrons. The energy equation describing the heavy particles would be similar to the energy equation for the electrons, however the Ohmic heating term would be absent. The electron energy equation and the heavy-particle energy equation are coupled to each other via the rate of electron energy loss per unit volume, due to collisions with heavy particles. In Equation 2.10, as in the conservation equations for momentum, the LHS represents convective terms, while the RHS describes the effects of thermal conduction in the axial and radial directions, viscous dissipation and Ohmic heating, respectively. Radiative losses are neglected. In Equation 2.10, e_T^* is given by $e^* + \rho^*(u^{*2} + v^{*2} + w^{*2})/2$ where e^* is the internal energy per unit volume given by $e^* = 3/2 n_T^* k_b T^* + \sum_{i=1}^{N_d} f_i^* n_i^* k_b T^*/2 + \sum_{i=1}^{N_d} \sum_{v=0}^{V_{max}} n_{i,v}^* E_{i,v}^* + \Delta\epsilon^*$. The $\Delta\epsilon$ term allows for the change of reference state (i.e. this term is the energy of formation per unit volume from chemical reactions or change in datum in molecular energy exchanges). The thermodynamic pressure, p^* is defined as $p^* = n_T^* k_b T^*$. In the energy equation, Φ^* is the dissipation function given by,

$$\begin{aligned} \Phi^* = 2 & \left[\left(\frac{\partial u^*}{\partial r^*} \right)^2 + \left(\frac{u^*}{r^*} \right)^2 + \left(\frac{\partial w^*}{\partial x^*} \right)^2 \right] + \left(\frac{\partial v^*}{\partial x^*} \right)^2 + \left(\frac{\partial u^*}{\partial x^*} + \frac{\partial w^*}{\partial r^*} \right)^2 \\ & + \left(\frac{\partial v^*}{\partial r^*} - \frac{v^*}{r^*} \right)^2 - \frac{2}{3} \left(\frac{\partial u^*}{\partial r^*} + \frac{u^*}{r^*} + \frac{\partial w^*}{\partial x^*} \right)^2, \end{aligned}$$

The equations describing the time evolution of the individual species (monatomic and diatomic) constituting the flowing gas are described next. Electronic states of monatomic and diatomic species are not considered in this work, although the present formulation allows their inclusion.

Species conservation equation for a monatomic specie is:

$$\begin{aligned} \frac{\partial n_m^*}{\partial t^*} + \frac{1}{r^*} \frac{\partial}{\partial r^*} (u^* n_m^* r^*) + \frac{\partial}{\partial x^*} (n_m^* w^*) + \frac{1}{r^*} \frac{\partial}{\partial r^*} \left(-r^* n_m^* \mu_m^* \bar{E}_r^* - \frac{r^* D_m^*}{k_b T^*} \frac{\partial}{\partial r^*} (n_m^* k_b T^*) \right) \\ + \frac{\partial}{\partial x^*} \left(-n_m^* \mu_m^* \bar{E}_x^* - \frac{D_m^*}{k_b T^*} \frac{\partial}{\partial x^*} (n_m^* k_b T^*) \right) = \dot{n}_m^* \end{aligned} \quad (2.11)$$

and for a diatomic specie is:

$$\begin{aligned} \frac{\partial n_{i,v}^*}{\partial t^*} + \frac{1}{r^*} \frac{\partial}{\partial r^*} (u^* n_{i,v}^* r^*) + \frac{\partial}{\partial x^*} (n_{i,v}^* w^*) \\ + \frac{1}{r^*} \frac{\partial}{\partial r^*} \left(-r^* n_{i,v}^* \mu_{i,v}^* \bar{E}_r^* - \frac{r^* D_{i,v}^*}{k_b T^*} \frac{\partial}{\partial r^*} (n_{i,v}^* k_b T^*) \right) \\ + \frac{\partial}{\partial x^*} \left(-n_{i,v}^* \mu_{i,v}^* \bar{E}_x^* - \frac{D_{i,v}^*}{k_b T^*} \frac{\partial}{\partial x^*} (n_{i,v}^* k_b T^*) \right) \\ = VT_{i,v} + VV_{i,v} + SRD_{i,v} + \dot{n}_{i,v}^* \end{aligned} \quad (2.12)$$

Detailed expressions for the VV, VT and the SRD terms are given in [12]. The terms $\dot{n}_m^*$ and $\dot{n}_{i,v}^*$ represent the net production of a particular component due to chemical reactions or molecular exchange processes.

2.3 Non-Dimensional Forms of the Governing Equations

The governing equations described in the previous section are solved in non-dimensional form. One advantage of doing so is that characteristic parameters of interest can be varied independently. Another is the control of round-off errors during the numerical calculation. The reference quantities used in this study are P_{ref} (a

reference pressure), T_{ref} (a reference temperature), l_{ref} (a reference length) and B_{ref} (based on the total current prescribed). All other non-dimensionalizing quantities can be normalized using these reference values.

The choice of l_{ref} is based on a characteristic length of the geometric configuration under study (a length or diameter). P_{ref} is usually the stagnation pressure. The reference temperature is chosen arbitrarily to be 10,000 K. The reference velocity is based on the isentropic speed of sound at the reference temperature. This choice of non-dimensionalization differs from convention (See section 5-1.6 of [10]) but is closely related to those used in [14]. Since, in general, the properties such as thermal conductivity and viscosity are locally varying (and in most instances by as much as orders of magnitude) in reacting flows, non-dimensionalization using quantities such as local frozen speed of sound [17], pressure etc., are neither useful nor relevant. From the foregoing definitions,

$$P_{ref} = n_{ref} k_b T_{ref} = \rho_{ref} R T_{ref}$$

$$u_{ref} = \gamma R T_{ref}$$

It must be pointed out here that γ in the above definition is not the ratio of the specific heats, but has a fixed value of 5/3. This arises as a result of expressing the internal energy e as the sum of the translational energies of all components (monatomic and diatomic) and the internal energies separately. For isentropic flows of a monatomic gas, γ is indeed equal to 5/3. In addition to these non-dimensionalizing factors, the magnetic transport equation is non-dimensionalized by B_{ref} , defined as

$$B_{ref} = \frac{\mu_0 I}{2\pi r_c}$$

where, I is the prescribed current and r_c is a dimension of the geometry under consideration.

Based on these non-dimensionalized quantities the governing equations after non-dimensionalizing are as follows: CONTINUITY EQUATION:

$$\frac{\partial \rho}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r}(r \rho u) + \frac{\partial}{\partial x}(\rho w) = 0 \quad (2.13)$$

RADIAL COMPONENT OF THE MOMENTUM EQUATION

$$\begin{aligned} \frac{\partial}{\partial t}(\rho u) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho u^2) + \frac{\partial}{\partial x}(\rho u w) - \frac{\rho v^2}{r} \\ = -\frac{3}{5} \frac{\partial p}{\partial r} + \frac{\partial}{\partial r} \left[2\eta \frac{\partial u}{\partial r} - \frac{2}{3} \eta \nabla \cdot \vec{u} \right] - (j_{\times} b) j_x B_{\theta} \\ + \frac{\partial}{\partial x} \left[\eta \left(\frac{\partial u}{\partial x} + \frac{\partial w}{\partial r} \right) \right] + \frac{2\eta}{r} \left(\frac{\partial u}{\partial r} - \frac{u}{r} \right) \end{aligned} \quad (2.14)$$

AZIMUTHAL COMPONENT OF THE MOMENTUM EQUATION

$$\begin{aligned} \frac{\partial}{\partial t}(\rho v) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho u v) + \frac{\partial}{\partial x}(\rho v w) - \frac{\rho u v}{r} \\ = \frac{\partial}{\partial r} \left[\left(\eta \frac{\partial v}{\partial r} - \frac{v}{r} \right) \right] + \frac{\partial}{\partial x} \left[\eta \frac{\partial v}{\partial x} \right] \\ + \frac{2\eta}{r} \left(\frac{\partial v}{\partial r} - \frac{v}{r} \right) \end{aligned} \quad (2.15)$$

AXIAL COMPONENT OF THE MOMENTUM EQUATION

$$\begin{aligned} \frac{\partial}{\partial t}(\rho w) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho u w) + \frac{\partial}{\partial x}(\rho w^2) \\ = -\frac{3}{5} \frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left[2\eta \frac{\partial w}{\partial x} - \frac{2}{3} \eta \nabla \cdot \vec{u} \right] \\ - (j_{\times} b) j_r B_{\theta} + \frac{1}{r} \frac{\partial}{\partial r} \left[\eta r \left(\frac{\partial u}{\partial x} + \frac{\partial w}{\partial r} \right) \right] \end{aligned} \quad (2.16)$$

where $j_{\times}b$ and η are defined as given below:

$$j_{\times}b = \frac{3}{5} \frac{B_{ref}^2}{\mu_o P_{ref}}$$

$$\eta = \frac{\eta^*}{l_{ref} u_{ref} \rho_{ref}}$$

The definition of non-dimensional viscosity, yields a non-dimensional Reynolds number equal to 1. The flows encountered in this study are characterized by varying properties and flow variables. Hence it is inappropriate to define a single Reynolds number characterizing the system. However, the Reynolds number based on typical velocities and viscosities yield values less than a 100, since the mass-flow rate is low (less than a few hundred milligrams). The low Reynolds number encountered in these flows justifies the assumption of laminar flow.

ENERGY EQUATION:

$$\begin{aligned} \frac{\partial e_T}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} \left(\left[e_T + \frac{2}{3} p \right] ur \right) + \frac{\partial}{\partial x} \left(\left[e_T + \frac{2}{3} p \right] w \right) \\ = \frac{1}{r} \frac{\partial}{\partial r} \left(kr \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) \\ + \frac{10}{9} \eta \Phi + j_{sq} \left(\frac{j_r^2 + j_x^2}{\sigma} \right) \\ + (j_{u \times} b) j_r w B_{\theta} - (j_{u \times} b) j_x u B_{\theta} \end{aligned} \quad (2.17)$$

In the energy equation, the thermal conductivity k is defined as

$$k = \frac{2}{3} \frac{k^*}{n_{ref} k_b u_{ref} l_{ref}};$$

and

$$\begin{aligned} e_T = n_T T + \sum_{i=1}^{N_d} \frac{f_i n_i T}{2} + \sum_{i=1}^{N_d} \sum_{v=0}^{V_{max}} n_{i,v} E_{i,v} \\ + \Delta \epsilon + \frac{10}{9} \frac{\rho (u^2 + v^2 + w^2)}{2} \end{aligned} \quad (2.18)$$

here,

$$f_i = \frac{2}{3} \frac{f_i^* l_{ref}}{P_{ref} u_{ref}}$$

$$E_{i,v} = \frac{2}{3} \frac{E_{i,v}^* l_{ref}}{P_{ref} u_{ref}}$$

$$\epsilon = \frac{2}{3} \frac{\Delta \epsilon^* l_{ref}}{P_{ref} u_{ref}}$$

j_{sq} is defined as

$$j_{sq} = \frac{2}{3} \left(\frac{B_{ref}}{\mu_o l_{ref}} \right)^2 \left(\frac{l_{ref}}{P_{ref} u_{ref}} \right)$$

and $j_{u \times b}$ is defined as

$$\frac{2}{3} \left(\frac{B_{ref}^2}{\mu_o P_{ref}} \right)$$

Non-dimensional form of the continuity equation for monatomic species is

$$\begin{aligned} \frac{\partial n_m}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (u n_m r) + \frac{\partial}{\partial x} (n_m w) + \frac{1}{r} \frac{\partial}{\partial r} \left(-r n_m \mu_m \bar{E}_r - \frac{r D_m}{kT} \frac{\partial}{\partial r} (n_m kT) \right) \\ + \frac{\partial}{\partial x} \left(-n_m \mu_m \bar{E}_x - \frac{D_m}{kT} \frac{\partial}{\partial x} (n_m kT) \right) = \bar{n}_m \end{aligned} \quad (2.19)$$

and the diatomic species is

$$\begin{aligned} \frac{\partial n_{i,v}}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (u n_{i,v} r) + \frac{\partial}{\partial x} (n_{i,v} w) + \frac{1}{r} \frac{\partial}{\partial r} \left(-r n_{i,v} \mu_{i,v} \bar{E}_r - \frac{r D_{i,v}}{kT} \frac{\partial}{\partial r} (n_{i,v} kT) \right) \\ + \frac{\partial}{\partial x} \left(-n_{i,v} \mu_{i,v} \bar{E}_x - \frac{D_{i,v}}{kT} \frac{\partial}{\partial x} (n_{i,v} kT) \right) = \overline{VT}_{i,v} + \overline{VV}_{i,v} + \overline{SRD}_{i,v} + \bar{n}_{i,v} \end{aligned} \quad (2.20)$$

In the monatomic and diatomic species, the $\bar{E}_r$ and $\bar{E}_x$ are defined as

$$E_r = \frac{B_{ref} j_r}{\mu_o l_{ref} u_{ref} \sigma}$$

$$E_x = \frac{B_{ref} j_x}{\mu_o l_{ref} u_{ref} \sigma}$$

$\bar{n}_{i,v}$ and $\bar{n}_m$ represent the non-dimensional net rate of production of the i^{th} species in the v^{th} vibrational state and the m^{th} monatomic species, respectively. The forward and backward rates describing these reactions are suitably redefined so that the nondimensionalizing multiplying factors are “absorbed” into the expressions describing the rates.

2.4 Magnetic Transport Equation

Maxwell’s equations are used to describe the B-field distribution established due to current flow through the plasma. The Ohmic heating term in the energy equation and the body force terms in the momentum equations are computed from the B-field distribution. A single equation for magnetic transport can be obtained from Maxwell’s equations [18] and Ohm’s law as follows:

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\nabla \times \vec{B} = \mu_o \vec{j}$$

$$\nabla \cdot \vec{B} = 0$$

In addition to the above set of equations, a relationship between $\vec{j}$ and $\vec{E}$ given by Ohm’s law

$$\vec{j} = \sigma [\vec{E} + \vec{u} \times \vec{B}]$$

is used to obtain the magnetic transport equation.

Elimination of $\vec{E}$ and $\vec{j}$ from these equations gives the magnetic transport equation in terms of $\vec{B}$ and σ as:

$$\nabla \times \left(\nabla \times \vec{B} \right) - \frac{\nabla \sigma}{\sigma} \times \left(\nabla \times \vec{B} \right) - \mu_o \sigma \left(\nabla \times \left(\vec{u} \times \vec{B} \right) \right) = 0 \quad (2.21)$$

where $\partial \vec{B}/\partial t$ term has been neglected.

The inclusion of the $\mu_o \sigma \left(\frac{\partial \vec{B}}{\partial t} \right)$ would involve resolution of extremely small time-scale due to the presence of the $1/c$ term in the unsteady magnetic transport equation. This would make the scheme unduly computation intensive and hence render it unattractive. This sort of computation is also unnecessary as a steady-state solution is desired. The assumption that the magnetic field relaxes to its new distribution instantaneously in each time step allows the exclusion of the time-derivative in the magnetic transport equation.

Using the vector identity

$$\nabla \times (\nabla \times \vec{B}) = -\nabla^2 \vec{B} + \nabla (\nabla \cdot \vec{B}) \quad (2.22)$$

and that $\nabla \cdot \vec{B} = 0$, equation 2.21 can be written as

$$-\nabla^2 \vec{B} - \frac{\nabla \sigma}{\sigma} \times (\nabla \times \vec{B}) - \mu_o \sigma (\nabla \times (\vec{u} \times \vec{B})) = 0 \quad (2.23)$$

The cross products in the above equations are expanded assuming that the magnetic field has only one component in the azimuthal direction, i.e. $\vec{B} = -\hat{e}_\theta B_\theta$.

The magnetic transport equation written in strong conservation form is as follows:

$$\frac{1}{r} \frac{\partial}{\partial r} \left(\frac{r}{\sigma} \frac{\partial B_\theta}{\partial r} \right) + \frac{\partial}{\partial x} \left(\frac{1}{\sigma} \frac{\partial B_\theta}{\partial x} \right) + \frac{B_\theta}{r} \frac{\partial}{\partial r} \left(\frac{1}{\sigma} \right) + \mu_o \frac{\partial}{\partial x} (w B_\theta) - \mu_o \frac{\partial}{\partial r} (u B_\theta) = 0 \quad (2.24)$$

Written in non-dimensional form

$$\frac{1}{r} \frac{\partial}{\partial r} \left(\frac{r}{\sigma} \frac{\partial B_\theta}{\partial r} \right) + \frac{\partial}{\partial x} \left(\frac{1}{\sigma} \frac{\partial B_\theta}{\partial x} \right) + \frac{B_\theta}{r} \frac{\partial}{\partial r} \left(\frac{1}{\sigma} \right) + \alpha \frac{\partial}{\partial x} (w B_\theta) - \alpha \frac{\partial}{\partial r} (u B_\theta) = 0 \quad (2.25)$$

where α is defined as $\mu_o u_{ref} l_{ref}$. In terms of the classical magnetic Reynolds number, $\alpha = R_m/\sigma$. Since the magnetic Reynolds number in the problems studied in the

present work are small, the $\vec{v} \times \vec{B}$ terms are neglected and the above equation is written as

$$\frac{1}{r} \frac{\partial}{\partial r} \left(\frac{r}{\sigma} \frac{\partial B_\theta}{\partial r} \right) + \frac{\partial}{\partial x} \left(\frac{1}{\sigma} \frac{\partial B_\theta}{\partial x} \right) + \frac{B_\theta}{r} \frac{\partial}{\partial r} \left(\frac{1}{\sigma} \right) = 0 \quad (2.26)$$

The above form of the magnetic transport equation is used in the computation of the B_θ in the present study.

2.5 Transport Properties

The governing equations discussed in the previous section include transport coefficients, namely, the coefficients of viscosity (η), thermal conductivity (k) and the species diffusivities ($D_{i,v}$ and D_m). In addition, the magnetic transport equation involves electrical conductivity (σ). These transport properties are evaluated using mean-free-path theory, wherein macroscopic quantities are calculated from kinetic theory [9]. The high number density in the plasmas under consideration ensures that microscopic processes are collision dominated. This justifies the use of the mean-free-path theory. The transport properties based on the mean-free-path theory depend on average cross-sections, number densities of the species, and temperature. Since these quantities have a spatial dependence, the properties also vary spatially. The electrical resistivity is calculated as the sum of an electron-neutral component and a Spitzer-Harm Coulomb component. In the present work, we use a conductivity “floor” in order to avoid instabilities associated with the calculation of the B-field. In the colder regions of the plasma flow, the electrical conductivity predicted by mean-free-path theory is plausibly less than the real electrical conductivity. The low conductivity in these regions makes the elliptical magnetic transport equation loose

the highest order derivative and hence, diagonal dominance. In practice, this conductivity floor is not an adjustable parameter. Rather it has a fixed value based on the total power, which is normally maintained during an experimental measurement. The value of the conductivity floor required to attain a specified power level is higher than that required for stability.

The drawback with the use of properties computed from mean-free-path theory is the reliance on average values of collision frequencies. These collision frequencies are in turn averaged over particle velocities. This averaging leads to results being accurate only to within a factor of two or three [9]. Computation of transport properties based on the EEDF gives more realistic estimates in non-equilibrium plasma flows.

2.6 Initial Conditions

The governing equations described in the previous sections are mixed hyperbolic-parabolic in character and it is important to specify appropriate initial conditions. The initial conditions for each of the variables are dependent on the problem at hand. These initial conditions will be further discussed with each case study. No initial distribution is required for the magnetic transport equation as it is elliptic in nature. However, the presence of the electrical conductivity in the magnetic transport equation indirectly demands an appropriate initial guess for the number densities and temperatures for stability.

2.7 Boundary Conditions

Solution of the governing equations described in the previous sections require the specification of appropriate boundary conditions for each of the dependent variable.

The boundary conditions are problem specific and will be discussed in detail with each case study. No-slip boundary conditions are applied for all components of velocity on the solid surfaces. Number densities are obtained by setting their second derivative to zero (i.e. $\partial^2\phi/\partial x^2 = 0$, where ϕ represents any variable). The magnetic transport equation also requires the specification of boundary conditions, which again will be discussed on a case specific basis.

The complete set of governing equations, and boundary and initial conditions constitute a model describing a particular phenomena or system. The solution of these equations yields variations of the quantities of interest describing the system. The complex form of the equations describing reacting plasma flows precludes analytical solution, leaving one with no recourse but to use numerical methods to obtain solutions. Chapter III describes the numerical technique employed in this work and its extension to the solution of reacting flows.

CHAPTER 3

NUMERICAL METHOD

3.1 Introduction

Models of reacting flows describe the close interaction between several chemical and physical processes. This leads to numerous difficulties in the numerical solution of the governing equations. As mentioned in Chapters I and II, the governing equations describing such flows are time-dependent, non-linear and strongly coupled. Several methods have been devised to solve these equations. The *Block-Implicit method* or *Global-Implicit method*, and the *Fractional Step method* or *Timestep Splitting* are two well known lines of approach. In the past, several attempts have been made to solve the compressible Navier-Stokes equations which essentially form a subset of the governing equations describing reacting flows. Among more popular methods of solving the compressible Navier-Stokes equations are MacCormack's Scheme[19], Beam-Warming's Scheme[20] and the Linearized Block Implicit Scheme of Briley and McDonald [14]. In this work, the *Linearized Block Implicit Scheme* developed by Briley and McDonald for the solution of the unsteady, compressible Navier-Stokes equations is extended to study *reacting flows*.

3.2 Block Implicit Methods

As explained in Chapter I, the choice of the time marching scheme, namely implicit or explicit, depends on the time-scales involved in the problem. Explicit methods are best suited for problems when the time-scales of interest are smaller than the minimum time-step dictated by the Courant condition. Simplicity in implementation is the single most important factor weighing in favor of explicit methods. However, if the time-scales of concern are greater than those required by the Courant condition ($\Delta t \leq \Delta x/c$) [21], and the equations are stiff, implicit methods have to be used. The reason is that stiffness precludes taking the maximum possible Δt allowed by the Courant condition. This makes the use of explicit schemes impractical as the computational time required for the solution of such equations is immense. If the equations are very stiff, then the size of the time-step required by explicit methods to resolve the fastest transient may be extremely small. In such situations, the size of the time-step may be comparable to the roundoff errors. Implicit schemes have the virtue of circumventing these problems, at a price, albeit. This price, is the complexity in the implementation of the algorithm. Implicit schemes involve the simultaneous solution of a system of equations. This either means an iteration procedure at each time step must be employed or complicated matrices must be inverted. This procedure requires greater computational effort as compared to explicit methods.

Implicit methods aimed at solving a coupled set of equations are known as Block-Implicit methods. Block-Implicit methods were developed by Lindemuth and Killeen, McDonald and Briley, Beam and Warming, Briley and McDonald [7] for solving compressible, time-dependent Euler and Navier-Stokes equations. The method essentially consists of a implicit scheme in which the solution is linearized by a Taylor expansion

about the value at the previous time level. This produces a set of coupled linear difference equations which are valid for a given time step. This procedure will be described in detail next.

A non-linear set of coupled partial differential equations can be written as [7]:

$$\frac{\partial y_i(x_j, t)}{\partial t} = G_i(y_j, \partial y_j / \partial x_i, \partial^2 y_j / \partial x_i^2, x_j, t) \quad (3.1)$$

where, y_i are elements of $\mathbf{y}$, a vector consisting of all the dependent variables and x_i are elements of $\mathbf{x}$, a vector denoting the spatial coordinate. Each element of the vector $\mathbf{y}$ is time-dependent. The block-implicit method treats each of the dependent variables using fully implicit finite-difference approximations. The right hand side of equation 3.1 is evaluated using quantities at the advanced time level. Equation 3.1 in finite-difference form can be written as:

$$\frac{\mathbf{y}^{n+1} - \mathbf{y}^n}{\Delta t} = \mathbf{G}^{n+1}$$

The arguments of $\mathbf{y}$ and G are suppressed in the above finite-difference equation for clarity. The above equation can also be written in the following approximate form:

$$\mathbf{y}^{n+1} \approx \mathbf{y}^n + \Delta t \mathbf{G}^{n+1} \quad (3.2)$$

The difficulty with the implicit treatment of the right hand side of equation 3.2 is that the new values of G depends on the values of y_j at the time level $n + 1$ which are unknown. Equation 3.2 could be solved either iteratively at each time step or *linearized locally about the solution at the previous time step and thus solved without iteration as done in the linearized block implicit schemes*. In principle, the solution of nonlinear difference equations obtained iteratively is attractive as it obliterates errors occurring due to the linearization process. However, iterative solution of nonlinear

difference equations can be very time consuming. Also, the convergence of the iteration is greatly dependent on the initial conditions prescribed. Hence from the point of view of stability and computational time, the later approach is advantageous.

The linearization of the nonlinear terms on the RHS of equation 3.2 is accomplished by assuming that the changes in y_j are small. If the changes in y_j are small then it may be assumed that the corresponding changes in G are small too. This assumption permits one to expand G^{n+1} in a Taylor expansion retaining only the first order terms in Δt . Thus yielding the form,

$$G^{n+1} = G^n + \Delta \mathbf{y} \frac{\partial G^n}{\partial \mathbf{y}}$$

The linearization procedure is illustrated in a lucid manner by applying the above technique to the one-dimensional continuity equation, which is of the form,

$$\rho_t + F_x = 0 \quad (3.3)$$

where F is ρu . Linearizing the above equation at time level $n + 1/2$ (Crank-Nicolson differencing) and at a spatial location j gives;

$$\frac{\rho_j^{n+1} - \rho_j^n}{\Delta t} + \left(\frac{\partial F}{\partial x} \right)_j^{n+\frac{1}{2}} = 0 \quad (3.4)$$

The subscript j denotes the spatial location of discretization. $\Delta t = t^{n+1} - t^n$. The changes in the dependent variables are assumed to be small in the time interval Δt .

The term $(\partial F / \partial x)_j^{n+\frac{1}{2}}$ is expanded as follows:

$$\left(\frac{\partial F}{\partial x} \right)_j^{n+\frac{1}{2}} = \left(\frac{\partial F}{\partial x} \right)_j^n + \frac{1}{2} \Delta t \left[\frac{\partial}{\partial t} \left(\frac{\partial F}{\partial x} \right) \right]_j^n + O(\Delta t)^2 \quad (3.5)$$

The term $\partial / \partial t (\partial F / \partial x)$ in the previous equation can be written as,

$$\frac{\partial}{\partial t} \left(\frac{\partial F}{\partial x} \right) = \frac{\partial}{\partial x} \left(\frac{\partial F}{\partial t} \right) = \frac{\partial}{\partial x} \left(\frac{\partial F}{\partial \rho} \frac{\partial \rho}{\partial t} + \frac{\partial F}{\partial u} \frac{\partial u}{\partial t} \right) = \frac{\partial}{\partial x} \left(u \frac{\partial \rho}{\partial t} + \rho \frac{\partial u}{\partial t} \right) \quad (3.6)$$

The equations 3.4 and 3.6 can be combined to give the following equation;

$$\begin{aligned} & \frac{\rho_j^{n+1} - \rho_j^n}{\Delta t} + \frac{u_{j+1}^n (\rho_{j+1}^{n+1} - \rho_{j+1}^n) - u_{j-1}^n (\rho_{j-1}^{n+1} - \rho_{j-1}^n)}{4\Delta x} + \\ & \frac{\rho_{j+1}^n (u_{j+1}^{n+1} - u_{j+1}^n) - \rho_{j-1}^n (u_{j-1}^{n+1} - u_{j-1}^n)}{4\Delta x} = \frac{(\rho u)_{j+1}^n - (\rho u)_{j-1}^n}{2\Delta x} \end{aligned} \quad (3.7)$$

In equation 3.7 central spatial differencing is used. This makes the scheme second order accurate in space. Even though equation 3.5 is linearized to second order, terms such as $\partial\rho/\partial t$ in equation 3.6 are forward differenced in time, which makes the overall scheme first order time accurate. Hence the truncation error for the scheme is $O[\Delta t, (\Delta x)^2]$. At steady-state the accuracy of the above scheme is $O[(\Delta x)^2]$. Equation 3.7 is unconditionally stable. It can be seen that equation 3.7 is linear in the quantity $(\rho^{n+1} - \rho^n)$ and all other quantities are known as they are evaluated at the time instant n .

In a system of coupled difference equations, each one of the equations is finite differenced in a manner akin to that illustrated above. In each of these equations, fully-implicit finite-differencing gives rise to terms such as, $(\phi_{1,j}^{n+1} - \phi_{1,j}^n)$, $(\phi_{2,j}^{n+1} - \phi_{2,j}^n)$, $(\phi_{3,j}^{n+1} - \phi_{3,j}^n)$, $\dots$, $(\phi_{q,j}^{n+1} - \phi_{q,j}^n)$, $(\phi_{1,j-1}^{n+1} - \phi_{1,j-1}^n)$, $(\phi_{2,j-1}^{n+1} - \phi_{2,j-1}^n)$, $(\phi_{3,j-1}^{n+1} - \phi_{3,j-1}^n)$, $\dots$, $(\phi_{q,j-1}^{n+1} - \phi_{q,j-1}^n)$, $(\phi_{1,j+1}^{n+1} - \phi_{1,j+1}^n)$, $(\phi_{2,j+1}^{n+1} - \phi_{2,j+1}^n)$, $(\phi_{3,j+1}^{n+1} - \phi_{3,j+1}^n)$, $\dots$, $\dots$, $(\phi_{q,j+1}^{n+1} - \phi_{q,j+1}^n)$, etc. and terms evaluated at the time instant n . It is assumed that the solution vector $\boldsymbol{\rho}$ in the above coupled set of equations contains q dependent variables. Terms such $\phi_{1,j} \dots \phi_{q,j}$ represent the various dependent variables constituting the vector $\boldsymbol{\rho}$ at the spatial location j , etc.. The quantities evaluated at time instant n are carried over to the right hand side of the individual equations and constitute the “source” terms. In other words, the fully-implicit finite-differencing of the q governing equations at the spatial location j following the Briley-McDonald method would

yield a set of linear algebraic equations as shown below

$$b_{11}\Delta\phi_{1,j-1} + \cdots + b_{1q}\Delta\phi_{q,j-1} + d_{11}\Delta\phi_{1,j} + \cdots + d_{1q}\Delta\phi_{q,j} +$$

$$a_{11}\Delta\phi_{1,j+1} + \cdots + a_{1q}\Delta\phi_{q,j+1} = s_{1,j}$$

$$b_{21}\Delta\phi_{1,j-1} + \cdots + b_{2q}\Delta\phi_{q,j-1} + d_{21}\Delta\phi_{1,j} + \cdots + d_{2q}\Delta\phi_{q,j} +$$

$$a_{21}\Delta\phi_{1,j+1} + \cdots + a_{2q}\Delta\phi_{q,j+1} = s_{2,j}$$

$\vdots$

$$b_{q1}\Delta\phi_{1,j-1} + \cdots + b_{qq}\Delta\phi_{q,j-1} + d_{q1}\Delta\phi_{1,j} + \cdots + d_{qq}\Delta\phi_{q,j} +$$

$$a_{q1}\Delta\phi_{1,j+1} + \cdots + a_{qq}\Delta\phi_{q,j+1} = s_{q,j}$$

The quantities $(\phi_{1,j}^{n+1} - \phi_{1,j}^n)$ etc. at each spatial location j , $j+1$, $j-1$, etc. are written as $\Delta\phi_{1,j}$, $\Delta\phi_{1,j-1}$, $\Delta\phi_{1,j+1}$, etc. This system of equations can be written in a compact form at each spatial grid point j as,

$$\mathcal{B}_j^n \psi_{j-1}^* + \mathcal{D}_j^n \psi_j^* + \mathcal{A}_j^n \psi_{j+1}^* = \mathcal{S}_j^n \quad (3.8)$$

where, ψ_j^* represents a vector comprising the incremental changes in the dependent quantities at successive time steps, at the spatial location j , i.e.,

$$\psi_j^* = [(\phi_{1,j}^{n+1} - \phi_{1,j}^n), (\phi_{2,j}^{n+1} - \phi_{2,j}^n) + \cdots + (\phi_{q,j}^{n+1} - \phi_{q,j}^n)]^T$$

$\mathcal{B}_j^n$, $\mathcal{D}_j^n$, $\mathcal{A}_j^n$, are square matrices each containing terms evaluated at the known time instant n at the spatial location j . $\mathcal{S}_j^n$, represents the vector comprising of the

source terms in each of the q equations at the spatial location j . The forms of $\mathcal{B}_j^n$, $\mathcal{D}_j^n$, $\mathcal{A}_j^n$ and $\mathcal{S}_j^n$ are given below.

$$\begin{aligned}
B_j &= \begin{bmatrix} b_{1,1,j} & b_{1,2,j} & \cdots & b_{1,q,j} \\ b_{2,1,j} & b_{2,2,j} & \cdots & \vdots \\ \ddots & \ddots & \ddots & \ddots \\ b_{q,1,j} & b_{q,2,j} & \cdots & b_{q,q,j} \end{bmatrix} \\
D_j &= \begin{bmatrix} d_{1,1,j} & d_{1,2,j} & \cdots & b_{1,q,j} \\ d_{2,1,j} & d_{2,2,j} & \cdots & \vdots \\ \ddots & \ddots & \ddots & \ddots \\ d_{q,1,j} & d_{q,2,j} & \cdots & d_{q,q,j} \end{bmatrix} \\
A_j &= \begin{bmatrix} a_{1,1,j} & a_{1,2,j} & \cdots & a_{1,q,j} \\ a_{2,1,j} & a_{2,2,j} & \cdots & \vdots \\ \ddots & \ddots & \ddots & \ddots \\ a_{q,1,j} & a_{q,2,j} & \cdots & a_{q,q,j} \end{bmatrix} \\
\mathcal{S}_j^n &= \begin{bmatrix} s_{1,j} \\ s_{2,j} \\ s_{3,j} \\ \vdots \\ s_{q-1,j} \\ s_{q,j} \end{bmatrix}
\end{aligned}$$

It is computationally advantageous to solve the equations 3.8 in terms of these incremental changes (i.e. $\Delta\phi_{1,j}$, $\Delta\phi_{1,j-1}$, $\Delta\phi_{1,j+1}$), etc. rather than the dependent variable itself at the next time instant (i.e. ϕ^{n+1}), not only because it simplifies the difference equations but also because it reduces round-off errors. If the number of dependent variables is q , then the size of each of the matrices, $\mathcal{B}_j^n$, $\mathcal{D}_j^n$, $\mathcal{A}_j^n$, is $q \times q$.

When equation 3.8 is written out for all the points (in one direction) it yields a system of equations which can be cast in a matrix-vector form. This can be done by an appropriate treatment of the boundary points using the boundary conditions.

Equation 3.8, when written out explicitly at $j = 1$, gives rise to terms such as $(\phi_{1,0}^{n+1} - \phi_{1,0}^n)$, $(\phi_{2,0}^{n+1} - \phi_{2,0}^n)$, $(\phi_{3,0}^{n+1} - \phi_{3,0}^n)$, $\dots$, $(\phi_{q,0}^{n+1} - \phi_{q,0}^n)$. These quantities are expressed in terms of $(\phi_{1,1}^{n+1} - \phi_{1,1}^n)$, $(\phi_{2,1}^{n+1} - \phi_{2,1}^n)$, $(\phi_{3,1}^{n+1} - \phi_{3,1}^n)$, $\dots$, $(\phi_{q,1}^{n+1} - \phi_{q,1}^n)$ and $(\phi_{1,2}^{n+1} - \phi_{1,2}^n)$, $(\phi_{2,2}^{n+1} - \phi_{2,2}^n)$, $(\phi_{3,2}^{n+1} - \phi_{3,2}^n)$, $\dots$, $(\phi_{q,2}^{n+1} - \phi_{q,2}^n)$ using the boundary conditions.

Similarly, equation 3.8, when written out explicitly at $j = N$, gives rise to terms such as, $(\phi_{1,N+1}^{n+1} - \phi_{1,N+1}^n)$, $(\phi_{2,N+1}^{n+1} - \phi_{2,N+1}^n)$, $(\phi_{3,N+1}^{n+1} - \phi_{3,N+1}^n)$, $\dots$, $(\phi_{q,N+1}^{n+1} - \phi_{q,N+1}^n)$ which can be expressed in terms of $(\phi_{1,N}^{n+1} - \phi_{1,N}^n)$, $(\phi_{2,N}^{n+1} - \phi_{2,N}^n)$, $(\phi_{3,N}^{n+1} - \phi_{3,N}^n)$, $\dots$, $(\phi_{q,N}^{n+1} - \phi_{q,N}^n)$ and $(\phi_{1,N-1}^{n+1} - \phi_{1,N-1}^n)$, $(\phi_{2,N-1}^{n+1} - \phi_{2,N-1}^n)$, $(\phi_{3,N-1}^{n+1} - \phi_{3,N-1}^n)$, $\dots$, $(\phi_{q,N-1}^{n+1} - \phi_{q,N-1}^n)$.

This enables the elimination of $\mathcal{B}_1$, and $\mathcal{A}_N$ from the system of equations. Thus, after elimination of the boundary conditions as described above, equation 3.8 at points $j = 1$ and $j = N$, are;

$$\mathcal{D}_1^n \psi_1^* + \mathcal{A}_1^n \psi_2^* = \mathcal{S}_1^n$$

$$\mathcal{B}_N^n \psi_{N-1}^* + \mathcal{D}_N^n \psi_N^* = \mathcal{S}_N^n$$

This system of equations given by (3.8) can now be written in a matrix-vector form as

$$\mathcal{C}\Psi = \mathcal{S} \quad (3.9)$$

where,

$$\mathcal{C} = \begin{bmatrix} \mathcal{D}_1 & \mathcal{A}_1 & 0 & \dots & 0 \\ \mathcal{B}_2 & \mathcal{D}_2 & \mathcal{A}_2 & & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & & \mathcal{B}_{N-1} & \mathcal{D}_{N-1} & \mathcal{A}_{N-1} \\ 0 & \dots & 0 & \mathcal{B}_N & \mathcal{D}_N \end{bmatrix}, \quad \Psi = \begin{bmatrix} \psi_1^* \\ \psi_2^* \\ \psi_3^* \\ \vdots \\ \psi_{N-1}^* \\ \psi_N^* \end{bmatrix}, \quad \mathcal{S} = \begin{bmatrix} \mathcal{S}_1^n \\ \mathcal{S}_2^n \\ \mathcal{S}_3^n \\ \vdots \\ \mathcal{S}_{N-1}^n \\ \mathcal{S}_N^n \end{bmatrix}$$

This block-tridiagonal system can be solved very efficiently using methods discussed in [22]. A detailed treatment of the linearized block implicit scheme can be found in [14].

3.3 Alternate-Direction-Implicit (ADI) Technique

If the number of grid points in one direction is N_x , and the number of coupled equations to be solved at each spatial location is q , then the size of the block-tridiagonal matrix, C obtained by applying the LBI scheme at each spatial point in the computational domain, is $qN_x \times qN_x$. The nature of the block-tridiagonal matrix is such that the overall computational matrix is very sparse. The blocks on the diagonal, and adjacent to the diagonal of C are $q \times q$ in size. Direct inversion of a matrix obtained from such a system of equations is computationally very time consuming. The operation count for a system described above using direct inversion methods is on the order of $(N_x q)^3$ [22]. In case of multidimensional problems, wherein, one has N_x grid points in one dimension, (say r -direction in $r - \theta - z$ system, or x -direction in $x - y - z$ system, etc.) N_y grid points in the second dimension (say, z -direction in $r - \theta - z$, y -direction in $x - y - z$ direction etc.) the size of the computational matrix, C is $qN_x N_y \times qN_x N_y$. Moreover, the computational matrix will not have a block-tridiagonal structure.

From the discussion in the previous paragraph, it is seen that multidimensional problems put very stringent demands on computational resources in terms of storage and solution of the matrices arising by applying block-implicit methods. This is due to the fact that large sparse matrices have to be solved completely over the entire computational domain at each time step.

Demands on computational resources can be greatly reduced if one resorts to the Alternating-Direction Implicit or ADI method for multidimensional problems. This method, first derived by Peaceman and Rachford [23], is used in the numerical solution of multidimensional Partial Differential Equations (PDEs). *The basis of this method is to make the equations implicit along only one direction at a time.* This approximation, leads to the equations reducing to three-point relations along one direction. These equations can then be cast in a matrix-vector form akin to equation 3.9. The block-tridiagonal form of the resulting equation can be solved efficiently. The intermediate solution obtained along one direction is then used in the solution of the system of equations in the other direction. An attractive feature of this scheme is that it is unconditionally stable. It is only conditionally stable in 3-D problems when periodic boundary conditions are used. This procedure can be extended to 3-D problems as well. A detailed explanation of the ADI procedure is given in [24]. In this work, following Briley and McDonald [14] we adopt the Douglas-Gunn ADI scheme for the solution of the multidimensional system of equations.

The application of the Douglas-Gunn ADI scheme, to the system of equations discussed in Chapter II is demonstrated next using a simple set of coupled equations in 2-D.

Consider a system of equations in 2-D written as;

$$\frac{\partial \phi}{\partial t} = D_x(\phi) + D_y(\phi)$$

Here, $D_x(\phi)$, $D_y(\phi)$ represent spatial derivative operators. Applying the Crank-Nicholson differencing at time instant $n + 1/2$, yields the following form:

$$\left(I - \frac{\Delta t}{2}\mathcal{L}_x - \frac{\Delta t}{2}\mathcal{L}_y\right) (\phi^{n+1} - \phi^n) = \Delta t (D_x + D_y) \phi^n \quad (3.10)$$

where $\mathcal{L}$ implies $\partial D / \partial \phi$.

The LHS of the above equation can be approximately factorized as follows;

$$\left(I - \frac{\Delta t}{2} \mathcal{L}_x - \frac{\Delta t}{2} \mathcal{L}_y\right) (\phi^{n+1} - \phi^n) \approx \left(I - \frac{\Delta t}{2} \mathcal{L}_x\right) \left(I - \frac{\Delta t}{2} \mathcal{L}_y\right) (\phi^{n+1} - \phi^n)$$

Equation 3.10 can then be written as

$$\left(I - \frac{\Delta t}{2} \mathcal{L}_x\right) \left(I - \frac{\Delta t}{2} \mathcal{L}_y\right) (\phi^{n+1} - \phi^n) = \Delta t (D_x + D_y) \phi^n \quad (3.11)$$

The above equation can also be written as

$$\left(I - \frac{\Delta t}{2} \mathcal{L}_x\right) \phi^* = R^n \quad (3.12)$$

where

$$\left(I - \frac{\Delta t}{2} \mathcal{L}_y\right) (\phi^{n+1} - \phi^n) = \phi^* \quad (3.13)$$

and,

$$R^n = \Delta t (D_x + D_y) \phi^n \quad (3.14)$$

Equation 3.12 is first solved to yield ϕ^* . Equation 3.13 is then solved to obtain the $(\phi^{n+1} - \phi^n)$.

This technique is called *Operator-Splitting*. It can be seen from the above treatment that the technique can be easily extended to 3-D problems. The method of operator-splitting has effectively reduced equation 3.10 to one that requires solution of another intermediate equation to obtain ϕ^* , which is then used to yield $(\phi^{n+1} - \phi^n)$. As mentioned above, the two-step solution of equation 3.10 maintains the narrow-banded block-tridiagonal structure in each dimension (direction) and hence lends itself to be solved by efficient block-elimination methods. A virtue of this method of operator-splitting is that the intermediate solutions are consistent approximations to

$(\phi^{n+1} - \phi^n)$. This facilitates the use of physical boundary conditions applicable to $(\phi^{n+1} - \phi^n)$ for the solution of the intermediate equations (i.e. equations containing ϕ^*) without a serious loss of accuracy. It is for this reason that the LBI scheme using the Douglas-Gunn ADI procedure is called “Consistently split Linearized Block Implicit method”. Briley and McDonald give a detailed analysis of the application of this method to multidimensions citebriley77.

3.4 Salient features of the LBI scheme

The LBI scheme exploits the favorable stability properties of implicit schemes and thus improves computational efficiency by allowing larger time steps to be used when time marching unsteady, coupled equations as compared with explicit methods. This method is easily extendable to multidimensional problems. *The true import of this method, is its promise to lead to development of efficient, non-iterative solutions of coupled nonlinear multidimensional PDEs describing reacting flows.* The stability properties of this scheme allow time steps in the time marching scheme of unsteady coupled equations to be orders of magnitude larger than the maximum allowable time steps for conditionally stable methods as determined by the Courant-Friedrichs-Lewy (CFL) condition. This a great boon in the solution of stiff equations describing chemical kinetics in reacting flows. Briley et.al report [14] report that the computational cost per time step is only approximately twice that of most explicit methods for problems involving cold flows through 3-D rectangular ducts. However, it is highly dubious if explicit methods can yield solutions to plasma flow problems at all.

3.5 Artificial Dissipation

In advection dominated flows, central differencing of the spatial derivative leads to severe problems of spurious oscillations due to lack of numerical dissipation [25]. Numerical diffusion, which can be a major source of error in finite-difference calculations has the same effect as physical diffusion [7]. The effect of numerical diffusion is not only to bring about a damping of the solution (dissipation) but also to distort the phase relations between various waves (dispersion). The spurious oscillations caused by a lack of adequate artificial dissipation often causes the solution to become unstable by making quantities like mass density and temperature go negative. Artificial dissipation of some form is necessary [7, 14] in order to avoid these spurious oscillations and maintain positivity. Artificial dissipation in some form is also necessary to provide overall stability to the algorithm when boundary conditions are treated inaccurately, when the mesh spacing is coarse or in the presence of discontinuities [14]. Ref. [25] gives a detailed discussion on artificial dissipation.

The artificial dissipation term used by Briley [14] is of the form $\varepsilon_x \mathcal{D}_x^2 \phi$, where

$$\varepsilon_x = \begin{cases} \frac{|w|\Delta x}{2} - \frac{1}{Re}, & Re_{\Delta x} > 2 \\ 0, & Re_{\Delta x} < 2 \end{cases}$$

where, $Re_{\Delta x} = |w|\Delta x Re$, and $Re = \rho_r U_r L_r / \mu$. This formulation ensures that the local cell Reynolds number is always less than two. Dissipation is added only in the direction of axial velocity. Briley however points out that the form of the dissipation term is provisional and cautions against its general use.

The dissipation model used in this work is different from that used by Briley. Artificial dissipation in the form of a second derivative is added in the axial and radial direction to all the governing equations. The functional form of the dissipation

terms used in this work is $\varepsilon_x \mathcal{D}_x^2 \phi + \varepsilon_r \mathcal{D}_r^2 \phi$, where ϕ is ρ in the continuity equation, u, v, w in the radial, azimuthal and axial components of the momentum equations, respectively, T in the energy equation and $n_{i,v}$ or n_m (as the case may be) in the species equations. The dissipation term is treated implicitly just as all other terms, and thus contributes to both the source terms on the right hand side as well as the elements of the block-tridiagonal on the left hand side.

The coefficients ε_x and ε_r are chosen so as to ensure the positivity of all the dependent variables and minimize the effect of the term $\varepsilon_x \mathcal{D}_x^2 \phi + \varepsilon_r \mathcal{D}_r^2 \phi$ on the overall solution. Unfortunately, the functional forms of ε_x and ε_r are dependent on the problem under consideration. These forms and their impact on the accuracy of the solution are described in greater detail in Chapter V on illustrative examples.

3.6 Grid Generation

The governing equations described in Chapter II describe the variables of interest in the physical domain. Physical domains of interest in this study have complicated geometries, for instance, C-D nozzles with throat-to-exit area ratios ranging from 25 to 225. In such situations it is necessary to transform the governing equations and the relevant boundary condition describing the flow in the physical domain to the computational domain. This transformation from the physical domain to the computational domain requires the inclusion of the metrics of mapping in the differential equations. To facilitate the use of the reacting flow solver developed here at The Ohio State University to a wide variety of problems, the grid generation module is independent of the reacting flow solver. Since this work is primarily directed towards obtaining 2-D axisymmetric solutions of reacting flows, the grid generation module

currently in use, transforms a 2-D (more specifically, the r and z directions) physical domain of interest, into a rectangular computational domain. The grid generation module currently allows the usage of non-uniform grids in the radial direction only. Use of non-uniform grids is not greatly advantageous in the axial direction since no steep gradients are encountered, except in regions where the relatively cold gas traverses the arc. Additionally, use of uniform grids in the axial direction simplifies the transformed equations considerably and hence greatly reduces programming efforts. Non-uniform grids in the radial direction, however, allow a better resolution of phenomena occurring close to physical boundaries (electrodes, for example). The grid generation routine transforms the physical domain into a computational domain and evaluates the transformation derivatives. These transformation derivatives are then read by the flow solver. Non-uniform transformation from the physical to the computational domain can be brought about by transformations similar to those described by Anderson et. al [10]. It is important to point out that non-staggered grids are used in this study. In the present work, *uniform grids in both the axial and radial direction* are used to solve the transformed governing equations and boundary conditions.

A general cylindrical coordinate system which is axisymmetric is described by r and x where r is the radial direction and x is the axial direction. In flows through geometrical configurations such as a CD nozzle, the radii of the inner and outer edge of the nozzle varies axially. It is convenient to apply a transformation to the radial coordinate so that the governing equations can be solved on a uniformly spaced grid in the computational domain. In other words, we are transforming from $(r(x), x)$ in the physical domain to $(\xi(\zeta), \zeta)$ in the computational domain. The coordinate

transformations employed in this work are:

$$\xi = \frac{r - r_i}{r_o - r_i}$$

and

$$\zeta = x$$

and where, $r_i(x)$ is the inner radius, $r_o(x)$ is the outer radius of the geometrical configuration and x is the axial length. This transformation yields, $\zeta_r = 0$ and $\zeta_x = 1$. Thus, under this transformation

$$\frac{\partial}{\partial r} = \xi_r \frac{\partial}{\partial \xi} \quad (3.15)$$

$$\frac{\partial}{\partial x} = \xi_x \frac{\partial}{\partial \xi} + \frac{\partial}{\partial \zeta} \quad (3.16)$$

$$\frac{\partial^2}{\partial r^2} = \xi_r^2 \frac{\partial^2}{\partial \xi^2} + \xi_{rr} \frac{\partial}{\partial \xi} \quad (3.17)$$

$$\frac{\partial^2}{\partial x^2} = \xi_x^2 \frac{\partial^2}{\partial \xi^2} + 2\xi_x \frac{\partial^2}{\partial \xi \partial \zeta} + \frac{\partial^2}{\partial \zeta^2} + \xi_{xx} \frac{\partial}{\partial \xi} \quad (3.18)$$

These transformations are used to transform the governing equations from the real physical domain to a rectangular computational domain (see. Figure 3.1).

3.7 Extension of the LBI scheme to Reacting flows

The transformed governing equations along with the case specific boundary conditions (to be discussed in Chapter V) are time-discretized using second order accurate Crank-Nicolson differencing. The linearization of the nonlinear terms is done according to the procedure described in section 3.2 on block implicit methods. All terms

Figure 3.1: Transformation from Physical Domain to Computational Domain

containing the dependent variables are discretized implicitly, including those in the boundary conditions. Discretization of the equations describing the time evolution of the diatomic species requires special attention. The source term of this equation contains the VT, VV, SRD and the net rate of production due to chemical reactions, $\dot{n}_{i,v}$. The VT, VV and $\dot{n}_{i,v}$ introduce stiffness in the equations. These terms are expressed in terms of implicit quantities such as number densities and temperature. The rate constants used in these terms also depend on temperature. However, only the number densities and temperature are treated implicitly, the rate constants are treated explicitly, i.e. they are evaluated using temperature values from the previous time step. This is primarily due to the fact that the expressions for rate constants are experimentally obtained values usually fit to a curve. More importantly, the experimentally available information on rate constants do not cover the entire temperature range which one is likely to observe in different problems. Implicit treatment of the

rate constants in these governing equations would preclude the possibility of changing the rate models with ease. Quasi 1-D simulations describing nozzle flows with high degree of vibrational non-equilibrium [12] have shown that explicit treatment of rate constants do not adversely affect the overall stability of the numerical scheme. Furthermore, since we are interested in steady-state solutions, errors arising out of explicit treatment of the rates in the transient solution are not a matter of great concern.

Since this work is aimed at examining 2-D axisymmetric flows, the Douglas-Gunn ADI scheme is used to solve the transformed governing equations. The transformed operators are consistently “split” as explained in section 3.3, and then solved in each spatial direction, namely, x - direction and r - direction. The spatial derivatives of the dependent variables in the transformed equations in each coordinate direction are then discretized using second-order accurate central differences. Boundary conditions are used to eliminate the boundary points, thus reducing the system of linear algebraic equations to obtain a block-tridiagonal system of equations in each coordinate direction. The algebraic relationship between the mass density and the number densities renders the system linearly dependent. These equations can be made linearly independent if one number density, say, $n_{i=1,v=0}$ were to be expressed in terms of the mass density and all the remaining number densities at each spatial grid point. Thus the species continuity equation for $n_{i=1,v=0}$ would not be solved. Having obtained the block-tridiagonal matrices, the unsteady set of equations are time marched. Computations can be begun with an initial guess, or from an intermediate solution that has been previously advanced to a certain time level. Properties are calculated at each time step based on the solutions from the previous time step. The magnetic

transport equation is solved at each time-step during the time marching. This is necessary because the transient nature of temperature and number densities cause the electrical conductivity, and hence the magnetic induction to change. The magnetic transport equation is solved using an odd-even point Jacobi iterative scheme. Solution of this system of equations in each coordinate direction, yields quantities such as $\phi_j^{n+1} - \phi_j^n$ where ϕ_j denotes the vector of the dependent variables, at each grid point in the computational domain. This correction $(\phi_j^{n+1} - \phi_j^n)$ when added to the quantity ϕ_j^n yields the solution at the next time level $n + 1$ (i.e. ϕ_j^{n+1}). The solution is thus advanced until steady-state is reached.

CHAPTER 4

CODE VERIFICATION

The simplest method to verify codes is to compare numerical results against known analytical solutions. Very often, it is possible to reduce a complex set of governing equations to a relatively simple set by introducing certain assumptions and boundary conditions. Comparing the results of the simplified set of equations to known analytical solutions is one good way of verifying the veracity of the numerical results. Performing a 1-D simulation and comparing against known analytical results is another way to gain confidence in the numerical algorithm and code being used. However, simplified models or 1-D models are very often inadequate in describing complex phenomena. Under such circumstances, one has no recourse but to compare the results of the numerical simulations against experimental results. One has to exercise caution in interpreting and using experimental data for code validation. Harsh environments and lack of sophisticated diagnostic techniques can affect the accuracy of experimental results. This is especially true in the case of measurements related to plasma environments. Comparing the results of a simulation with sets of experimental measurements made using different techniques (where possible) is helpful in highlighting the merits and demerits of different measurement principles. In order to ensure that close agreement between the results of a numerical simulation

and experimental results are not fortuitous, one has to subject the model/code to a variety of test problems with widely varying conditions, and compare the results with experiments where possible. Elaborate investigations of this kind are perhaps the best way of validating the results of numerical simulations. However, care must be exercised in ensuring that comparisons between model and experiment are made on the same platform, i.e. under identical conditions. In the absence of experimental or analytical results for a given problem, one may have to be content with comparing the solutions obtained with those generated using other numerical schemes.

The complexity of the governing equations describing plasma flows makes it imperative to test the model and the code at every stage, in order to ensure accurate results. As mentioned in Chapter III, the algorithm used to study reacting plasma flows in this work is amenable to extension from quasi 1-D to 2-D and 3-D situations. Our efforts to develop a modular high-performance reacting flow code has progressed in stages of increasing complexity. Quasi 1-D cold flow simulations were performed on different geometrical configurations. The results of these simulations were compared with analytical solutions for isentropic flow. The next step involved the inclusion of state-specific kinetics in 1-D [12] and comparison with other published numerical models [13]. This was followed by 2-D axisymmetric cold flow simulations. Inclusion of the electromagnetics to simulate the presence of an arc in the 2-D axisymmetric formulation was the next step. These simulations have then been applied to a variety of cases. Internal flow simulations in arcjets with hydrogen as the propellant were studied for two different geometrical configurations corresponding to two different power levels - 30 KW [26] and 1 KW. These simulations include simple reactions in hydrogen, but disregard the role of internal modes of molecular motion. No analytical

solutions exist for these flows. In order to verify the accuracy of the results of our simulations, detailed comparisons have been made with experiments for the 1 KW arcjet geometry [27]. The 2-D axisymmetric flow simulations with inclusion of the arc have also been used to study internal and external flows in welding plasmas. The results of these simulations have been compared with available experimental data. These comparisons are discussed in detail in the next chapter on Illustrative Examples. These studies also serve the purpose of code validation, in part.

In this chapter, results for three case studies involving quasi 1-D flows are presented and compared with analytical solutions. The geometries in these simulations have an exit-to-throat area ratio of 10, 100 and 225 (1 KW arcjet geometry). These three case studies bring to fore the ability of the numerical scheme to handle widely varying geometric configurations and serve to identify the limits of the model's applicability. The area-ratio 10 and 100 configurations were each studied with two different grid-sizes (150 and 1500 grid-points) for two different values of γ (ratio of specific heats): 1.4 (diatomic gases) and 1.67 (for monatomic gases). The 1 KW arcjet geometry was studied for two different grid sizes (150 and 1500) for $\gamma = 1.4$. Direct comparison of the variation of Mach number obtained from these simulations with those predicted from analytical solutions for isentropic quasi 1-D flows based on the well-known Area-Mach number relation [10] are presented in the next section for each of the three cases. This chapter is concluded with a discussion of results and inferences that can be drawn on the basis of these comparisons.

4.1 Results

Figures 4.1, 4.2 and 4.3, show a comparison between values computed from the quasi 1-D code and isentropic relationships for Mach number for exit-to-throat area-ratios of 10, 100 and 225 respectively. The plots include the effects of different

Figure 4.1: Comparison of Analytical and Computed Results (Area-Ratio = 10)

grid-sizes and values for γ . The computed values match those obtained from isentropic considerations closely. The difference between the predicted values and theoretical

Figure 4.2: Comparison of Analytical and Computed Results (Area-Ratio = 100)

Figure 4.3: Comparison of Analytical and Computed Results (Area-Ratio = 225)

values are largest in the supersonic region near the exit plane (approximately 10% in the coarse grid case). It can be further seen that with a decrease in the grid spacing the discrepancy in the results is reduced. It is further observed that with increasing area-ratios the discrepancy between isentropic results and those obtained from simulations tend to increase. For a given area-ratio, the discrepancy is greater in the case with $\gamma = 1.67$ as compared with $\gamma = 1.4$. This is due to the fact that monatomic gases have at least two fewer degrees of freedom than diatomic gases, resulting in larger gradients in the flow in the diverging section.

4.1.1 Discussion of Results

It can be seen from the figures 4.1 through 4.3 that the agreement between analytical results and the computations are very good. The maximum discrepancy is about 10% for the case of coarse grids. This discrepancy arises due to the effect of artificial dissipation [28] and truncation errors. As pointed out in chapter III, the artificial dissipation term is of the form $\epsilon_x \partial^2 \phi / \partial x^2$, where ϵ_x is given by $0.5 \rho w dx$ and dx is the mesh spacing. As expected, in all the case studies, the effect of numerical dissipation is larger in the case with coarser grids. It must be pointed out that the analytical results for isentropic flow do not take into consideration the effects of friction. However, as pointed out in Chapter III, the LBI scheme requires the addition of artificial dissipation for stability of the time-marching procedure. Addition of artificial dissipation induces effects similar to viscous effects. It is well known that friction tends to decelerate supersonic flows. Temperatures obtained from quasi 1-D computations are higher as compared to those predicted for isentropic flows. Axial velocity computed by the quasi 1-D simulations are lower as compared to those predicted for isentropic

flows. Thus the Mach number computed from the quasi 1-D simulations are lower than those predicted by analytical solutions for isentropic flows. The influence of the dissipation term is highest in regions close to the exit plane, where the discrepancy between analytical results and results computed from quasi 1-D simulations is largest. Reducing ϵ_x by a factor of 10 only in the supersonic regions of the flow, in the nozzle geometry with exit-to-throat area-ratio of 10, reduced the discrepancy between the analytical and predicted results to less than 1%.

There is no unique method to specify the optimum amount of artificial dissipation at each point in the computational domain so as to maintain positivity and hence stability. This is a drawback of the numerical scheme used, however, it is seen that it does not affect the results of the simulation a great deal. Increasing the number of grid points for a given area ratio tends to improve the accuracy of the results. This is largely due to the fact that increasing the number of grid points reduces the effects of numerical dissipation which scales directly with the grid spacing (Δx). The effects of artificial dissipation are expected to be less pronounced in the solution of real viscous flows due to the presence of natural dissipation. However, the present code has the ability to provide results for quasi 1-D flow problems that converge to the 12th decimal in a matter of a few seconds to a few minutes of CPU time depending on the initial guess and number of grid points, on a Silicon Graphics Indigo Workstation. It is this efficiency feature of the LBI algorithm that makes it attractive for computations involving multi-dimensions and large coupled sets of governing equations.

Chapter V describes the complex case-studies to which the algorithm has been successfully applied. The results of these simulations are compared with experimental

data. These comparisons are another step in the validation of large codes used in the simulation of reacting plasma flows.

CHAPTER 5

ILLUSTRATIVE EXAMPLES

Reacting plasma flows occur in a wide variety of discharges. The conditions under which these discharges are operated, vary widely depending on the application. This work is primarily directed toward developing high-performance simulation tools to understand the physics of high-speed reacting plasma flows occurring in various discharges. Characteristics of discharges vary widely depending on the operating conditions, geometry and gaseous medium. Studying such discharges is of vital importance in evaluating the present numerical scheme and model. With this intent, the present work investigates plasma flows through arcjet thrusters and plasma torches. These two case studies have been chosen as they represent two technologically important areas, namely space propulsion and materials processing. Moreover, the operating conditions and configurations of these discharges make them ideal candidates for the next level of model and code validation.

Arcjet thrusters, used in space propulsion applications are relatively low-pressure discharges whereas the welding torches operate at higher pressures (near atmospheric). Plasma torches usually use argon as the plasma gas, whereas arcjet thrusters use molecular propellants such as Hydrogen (H_2), Ammonia (NH_3) or Hydrazine (N_2H_4).

Thus, plasma torches usually comprise of atomic plasmas whereas arcjets have a flowing molecular plasma stream. Arcjet thrusters consist of a C-D nozzle whereas plasma torches do not have a diverging section. The composition and pressure of the plasma stream greatly affects the electrical characteristics of the discharge. The availability of excellent experimental data from several groups enables comparisons to be made between models and experimental measurements. These comparisons serve to evaluate the strengths and weaknesses of the present model and numerical method.

This chapter is organized as follows. The background physics of electric discharges is discussed first before each illustrative case-study is described in detail. Such a discussion is necessary as the present work endeavors to develop a basic understanding of the interaction between ionized gas flow and electromagnetic fields. This is followed by a discussion of the assumptions made in this work. The next section discusses flows through hydrogen arcjets. No internal modes are considered in these simulations. Only a few relevant elementary reactions are included in these case-studies. This is followed by an investigation of internal and external flow through plasma torches. Each of these case-studies is described in subsections which provide the necessary background and relevance of the problem, problem formulation including governing equations, and boundary and initial conditions. In addition, operating parameters, results and comparisons of results with experimental data where available, and a detailed discussion of these results is included for each case-study.

5.1 Physics of Electric Discharges

All gases at room temperature are excellent electrical insulators. This is due to the fact that the number of charge carriers is very low ($\approx 10^6$ electrons/ m^3 or

less). However, these charge carriers are responsible for an electrical breakdown, if the gas were to be subjected to a sufficiently strong electric field. Electron-impact ionization is the most important mechanism responsible for the growth of the free-electron population in a gas subjected to an electric field. The energy gained by the electrons from the electric field results in ionization of neutral atoms and molecules. This is known as primary ionization and the electrons thus produced are known as primary electrons.

There are several mechanisms which produce secondary electrons. Impact of positive ions at the cathode surface is a major source. As the number of charged particles in the region subjected to the electric field increases beyond a threshold, breakdown of the gas occurs. Breakdown is said to occur when a discharge is initiated through the gas. It is dependent on the values of E/p , (where E is the electric field and p is the gas pressure) to which the gas is subjected. Electrical breakdown is well described by Townsend's theory [29] and occurs when a condition known as the Townsend criterion is satisfied. The Townsend criterion is given by

$$\gamma_T (e^{\alpha d} - 1) = 1$$

In the above equation, α is Townsend's first coefficient defined as the average number of electron-ion pairs created by an electron while traversing a distance of 1 cm, γ_T is Townsend's second coefficient defined as the number of secondary electrons ejected from the cathode after an ion strikes it and, d is the distance between the electrodes. The resulting gaseous discharges consists of a mixture of electrons, ions and neutral particles. The composition and distribution of the plasma depends on the discharge mode, and operating conditions such as gas pressure and electrode gap distance. The nature of the discharge is determined by its Voltage-Current (V-I) characteristics.

Figure 5.1: V-I Characteristics of a DC Discharge [30]

Figure 5.1 (from ref. [30]) shows a schematic of the various types of discharges that may occur in a discharge chamber with a gas pressure on the order of 0.1 kPa and an electrode gap of a few centimeters. The different types of discharges based on the V-I characteristics (see Fig 5.1) are described next.

(i) Townsend Discharge or Dark Discharge:

When a potential is applied across two electrodes, initially the current rises slowly in accordance with Ohm's Law. After reaching a certain value, the current stops rising while the voltage rises steeply. This region is known as the saturated current region. In these two regions the discharge is not self-sustaining, i.e. the discharge cannot continue without an external agent. Following these two regimes, is a region where the current continues to increase rapidly even

though the voltage remains nearly constant. This is the regime of the *Townsend discharge*. The current in this region of the discharge is low (less than 10^{-6} Amps) and there is practically no visible glow. This is why the region is also known as the dark discharge. The currents in this region of the discharge are typically between 10^{-10} A and 10^{-6} A and the $V \approx 10^3$ V for gap distances on the order of a few centimeters.

(ii) Glow Discharge:

In the region beyond the Townsend discharge, the V-I curve shows an unexpected characteristic. dV/dI and hence the dynamic resistivity, is negative in this region. This region is metastable. It is a transition zone between the Townsend discharge and the glow discharge region. The glow discharge region is characterized by increasing currents at a nearly constant voltage. The typical values of the voltages are approximately 100 V and the currents lie between 10^{-4} A and 10^{-2} A. This regime of the discharge is the one that is most extensively studied because of its utility in lighting, lasers and materials processing.

(iii) Arc Discharge:

In the last stage of the glow discharge, the V-I characteristics exhibit another metastable region. When the current is between 10^{-2} A and 1 A, the V-I characteristics show a region which obey Ohm's Law. This is followed by another region which has a negative dV/dI and hence a negative dynamic resistivity. Increasing the current beyond 1 A, the voltage drops and settles down to a steady value. This steady value of the voltage is independent of the current. In this region, the current can be varied from about 10 A to 1 KA, but the voltage

remains relatively constant in the range of tens of volts. This region is known as that of the *Arc Discharge*, and is characterized by low voltages and high currents. This region is also unique in that the electron temperatures are usually equal to the heavy particle temperature (except at the arc boundaries).

5.2 General assumptions in the modeling of electric discharges in this work

The discharges modeled in this work do not account for the electrode-adjacent or sheath regions. Although the formulation and methods used here do not preclude modeling of these regions, the arc (in this work) is assumed to comprise of the arc-column only. This assumption is justified since the sheath which is usually a few Debye-lengths thick would be typically on the order of a few microns or less in extent at ordinary pressures. This is negligible compared to the characteristic dimensions of problems under consideration. Moreover, the characteristics of these electrode-adjacent regions are not well-understood at this time and the inclusion of these regions in the simulation of the main body of the arc (i.e. the arc-column) would lead to complications in the solution of the problem (in terms of resolution and memory). The plasma is assumed to be quasi-neutral. This assumption is not valid in the sheath regions and hence should be modified when extending the present formulation to include the sheath regions. Excluding the sheath regions introduces little error in the general properties of the bulk of the plasma but does affect the computed values of the terminal voltage between the electrodes.

Flowing plasmas are treated as laminar (due to the low Reynolds numbers in the cases studied) and line radiation from the plasma is neglected. A single temperature model is used to describe both the heavy particles and the electrons. While this

is a reasonable assumption in the case of high pressure discharges where a higher number of elastic collisions ensures LTE, it is not entirely true in the case of low pressure discharges or plasmas in diatomic gases. This assumption is also not true in the fringes of high pressure arcs. Nevertheless, a single temperature model is the first step in the present ambitious attempt to obtain realistic models describing non-equilibrium plasma flows. Molecular plasmas are assumed to consist of electrons, atoms, molecules, atomic ions and molecular ions whereas atomic plasmas are considered to be a mixture of neutral atoms, singly-ionized atoms and electrons.

The above assumptions provide a framework to model plasmas. The governing equations described in Chapter II incorporate these assumptions and are used to model flows in arcjets and plasma torches. Arcjet thrusters with H_2 as the propellant is the first case study presented and plasma torches with Ar as the plasma gas is the second. The next two sections discuss arcjet thruster and plasma torches in greater detail, examining the issues associated with each of these devices. Results and comparisons with available experimental measurements are also presented.

5.3 Case Study I: Arcjet Flows

5.3.1 Introduction

Arcjet thrusters have primarily been targeted as low-power, high specific-impulse ($I_{sp} \approx 1000s$) propulsion devices. These thrusters are currently used for North-South Station Keeping (NSSK) of geosynchronous communication satellites. Arcjet thrusters impart directed kinetic energy to a propellant stream by Ohmically heating it and subsequently expanding to supersonic speeds. In addition to aerospace applications, these thrusters also have terrestrial applications in the area of materials

processing. Arcjets are used commercially in the growth of free-standing diamond films and coatings.

The device essentially comprises of an inlet plenum, a converging section, a straight portion called the constricter, followed by a diverging section or supersonic nozzle. The propellant enters the inlet plenum, relatively cold, un-ionized at subsonic speeds. The flow entering the plenum is, at times injected with swirl (which is believed by some) to stabilize the arc. This cold, un-ionized gas is rapidly heated by an arc discharge between the cathode and the anode, as a result of an electric field applied between the two electrodes. The heated gas reaches near-sonic speeds by the end of the constricter and then rapidly expands in the diverging section to supersonic speeds. The propellant could be one of the following gases - Molecular hydrogen (H_2), ammonia (NH_3), hydrazine (N_2H_4).

Molecular hydrogen, is an ideal propellant primarily from the I_{sp} vantage point, due to its low molecular weight. However, it presents considerable difficulty in terms of handling and storage in space. Ammonia and hydrazine are other potential candidates from the ease of storage point of view. However, the higher molecular weights of these propellants bring about a reduction in the I_{sp} . Another disadvantage of these polyatomic molecules is their tendency to produce diatomic molecules which “soak” up considerable input electrical energy in their internal modes such as vibration and rotation, thus reducing the amount of directed kinetic energy available at the exit plane of these thrusters. The hydrogen arcjet is considerably different from the ammonia and hydrazine arcjet. A single temperature model can describe the performance of H_2 arcjets reasonably well (as will be seen in the section on results). This is due to the fairly quick V-T relaxation of the vibrational modes of molecular

hydrogen by H atoms. However, such a single temperature description of discharges comprising molecules such as Nitrogen (N_2) would be incorrect. This is especially true in arcjet geometries that have low mass-flow rates and high velocities. Low densities and high velocities greatly reduce the rate of relaxation of the vibrational modes. An accurate description of arcjet configurations with high exit-to-throat area-ratios with a propellant stream consisting of molecules such as nitrogen would require the inclusion of a Boltzmann-like equation describing the EEDF in addition to an energy equation describing the evolution of energies of all the heavy particles.

The operating principle of an arcjet is deceptively simple, although, the physics governing the dynamics of the energy transfer from the arc to the gas flow and its subsequent acceleration, are only beginning to be understood. This is especially surprising since these thrusters are space-qualified and in fact, two 1.4 KW hydrazine arcjet thrusters have been operational on the Telstar IV communication satellite since December 1994. The operating thrust efficiency of these arcjets is only about 28% and improvement in thrust efficiency is highly desirable. The non-equilibrium nature of these flows result in frozen flow losses thus degrading the thrust efficiencies of these devices. Frozen flow losses refer to that portion of the input electrical energy which is lost to molecular processes such as dissociation, ionization, vibrational, rotational and electronic excitation. They are referred to as “frozen flow losses” since the energy trapped in these modes is not recovered as directed kinetic energy at the exit plane of the thruster. This happens when the convective time-scales of the flow are comparable to the relaxation times governing the various internal processes. The poor efficiency of arcjets directly affect mission costs and payload that can be carried (this is true for

any propulsion device). Hence the viability of these devices as low power propulsion devices, can be ensured only if some of these frozen flow losses can be recovered.

5.3.2 Background

Attempts to improve the overall thrust efficiency of arcjets requires a thorough understanding of the dynamics of energy transfer from the arc to the propellant stream. With the intent of gaining a deeper understanding of arcjets, several groups have embarked on experimental and computational studies. However, both approaches are fraught with difficulties. This is primarily due to the nature of the arc. The geometry of arcjets makes the arc primarily two-dimensional. In fact, it is very likely that the arc is three-dimensional in nature, when its attachment on the anode is asymmetrical. The location of the arc attachment is one of the least understood phenomena. Since the breakdown of the gas and the subsequent attachment of the arc depends on the details of its initiation, it is difficult to ensure attachment at a repeatable location. The axisymmetric nature of the arc can easily be lost due to uneven electrode erosion and/or initial mis-alignment of the electrodes. The arc attachment significantly influences the energy loading of the gas which in turn affects the species concentrations, velocity and the temperature fields in the arcjet. Due to these uncertainties in the arc attachment, experimental data have a considerable amount of scatter. In addition, experimentalists have to contend with harsh environments which makes reliable measurements a daunting task.

Numerical simulation of arcjet flows is also beset with difficulties. The two-dimensional nature of the arc renders 1-D analytical models largely incapable of

elucidating the intricate issues governing these flows. This necessitates the development of multidimensional models to gain a clearer understanding of the operation of these devices. Time-marching the governing equations describing flowing plasmas to steady-state is plausibly the best way to understand the physics governing arcjet flows. Schrade et.al.[31] have modeled two-dimensional, axisymmetric, fully ionized flow in MPD arcjets. The hybrid nature of MPD arcjets (electromagnetic/electrothermal) is of limited use in the study of arcjets which are purely electrothermal devices. The exclusion of the effects of finite-rate chemistry in their model is the main drawback of their work. Schrade et.al [32, 33] have also attempted to understand arc attachments and arc dynamics in the constrictor region. Their quasi one-dimensional, two-fluid model examined the interaction between the flow in the hot arc and the cooler outer flow in the constrictor region of the arc. Butler et. al. [34], King and Butler [35] and Rhodes and Keefer [36] have attempted to describe arcjet flows using two-temperature axisymmetric models. However, these models too lack the inclusion of chemical kinetics. Exclusion of chemical kinetics in these models makes them largely incapable of explaining the operation of arcjet thrusters.

Recently, however, more realistic simulations have been produced by some groups. Miller and Martinez-Sanchez [37] have produced the first two-temperature model of a Hydrogen arcjet in a 30 KW arcjet geometry (exit-to-throat ratio of 25). This study concluded that dissimilar heavy particle and electron temperature are encountered only in the supersonic diverging section. This conclusion though plausible for H_2 arcjets, is unlikely to give realistic description of flows in arcjets with ammonia or hydrazine as propellants. There are also other multi-temperature models describing

1 KW arcjet [36, 38], but these do not exhibit the computational performance necessary to include state-specific kinetics. The only model to-date that has studied flows in a N_2/H_2 arcjet is that of Megli, Krier, and Burton [39]. This is a steady, two-temperature model that includes finite-rate chemistry. This steady-state model decouples the energy equations (for electrons and heavy particles), chemical kinetics, momentum and electromagnetics from each other. In other words, the iterative scheme obtains a converged solution for T_e and T_h , which is then used in the chemical kinetics followed by the continuity and momentum equations and finally the electromagnetics. Moreover, the species equations do not include state-specific kinetics. The electron-molecule collision frequencies are multiplied by an energy loss factor δ to account for inelastic losses to the internal rotational, vibrational and electronic excitation energy modes. These modified collision frequencies are then used to evaluate the energy loss due to collisions between electrons and the heavy particles. This energy loss term is used in the electron energy and the heavy particle energy equations. However, there is a considerable degree of uncertainty associated with the energy loss factor δ which can vary up to three orders of magnitude [9]. The results obtained by such a formulation is greatly dependent on the value of δ [40] and can lead to large errors of state-specific concentrations.

The present work, in contrast to earlier work, is a systematic study, treating the flow equations, chemical kinetics and electromagnetics in a self-consistent manner. This self-consistent formulation confers a great deal of reliability upon the results of this work. At this point it must be stressed that a self-consistent formulation puts great demands on the numerical scheme and computing resources. The numerical

algorithm used in this work permits the combined treatment of chemical kinetics (including state-specific kinetics), electromagnetics and the flow equations. Extension of this method to investigate three-dimensional flows is an added advantage of the present scheme. However, such an extension to 3-D would limit the number of equations that can be included in the set of governing equations largely due to memory requirements.

The performance characteristics of a 1 KW H_2 Arcjet thruster are investigated in this work. This lays the foundation to solving the Electron-Energy- Distribution-Function (EEDF) in conjunction with the flow equations and state-specific kinetics. The effects of molecular propellants such as ammonia or hydrazine on arcjet performance would require a detailed model of this nature.

A knowledge of the electron energy distribution is helpful in elucidating the channels of energy transfer by which the input electrical energy is distributed to the various internal modes (most likely vibration) and the external mode (translational). This understanding may hold the key to the recovery of frozen flow losses in these devices. Having provided this background on arcjets, the next subsection describes the general formulation of the problem of internal flow in arcjets.

5.3.3 Formulation

The general conservation equations describing reacting plasma flows are described in Chapter II. The non-dimensional form of governing equations described in Chapter II (section 2.3) are adapted to the case describing H_2 arcjets and solved in conjunction

with the appropriate boundary and initial conditions to obtain the velocity, temperature and species concentration. These boundary and initial conditions are discussed next.

Boundary Conditions

At the inlet, the radial component of velocity, u , is set to zero, the azimuthal component v is usually set to a prescribed distribution to simulate swirl (or set to zero in the absence of swirl) and the axial component is evaluated by setting its second derivative to zero, i.e. $\partial^2 w / \partial x^2 = 0$. The swirl component of velocity is set to zero in the results presented here or else it too can be extrapolated. A stagnation pressure and stagnation temperature are prescribed at the inlet. Using the principle of conservation of energy, the temperature at the inlet plane can be obtained from the prescribed stagnation temperature and velocity:

$$T_o = T_{i=0} + \frac{u_{i=0}^2 + v_{i=0}^2 + w_{i=0}^2}{2C_p}$$

However, since u and v are both set to zero in the present study, the above equation is written as

$$T_o = T_{i=0} + \frac{w_{i=0}^2}{2C_p}$$

The inlet static pressure (and hence the number densities in cases involving multi-component gases) and temperature can be related to their respective stagnation values through the isentropic equation of state. The low velocities at the inlet plane allow the assumption of isentropy. Thus,

$$\frac{P_o}{P_{i=0}} = \left(\frac{T_o}{T_{i=0}} \right)^{\frac{\gamma}{\gamma-1}}$$

where $P_{i=0} = n_{T_{i=0}} k T_{i=0}$. This gives a relationship between the total number density ($\sum_{i=1}^{i=N} n_i$) and the temperature at the inlet plane. The number densities of all

the species except one are obtained by setting their second derivatives in the axial direction to zero. Knowing the total number density from the isentropic equation of state, the remaining number density can be obtained. Knowing the number densities of all the individual species, mass density at the inlet plane can be obtained via the relationship, $\rho = \sum_{i=1}^{i=N} m_i n_i$.

In case the propellant stream consists of a mixture of monatomic (diluent) and diatomic species, it is assumed that the total temperature, total pressure and the volume fraction of various species present are known at the inlet plane. The total number density is evaluated as described above. Knowing the volume fractions, individual monatomic species are obtained from the relation, $n_m = X_m n_T$, where X_m is the volume fraction of the m^{th} monatomic species. Similarly, the i^{th} diatomic species is obtained from the relationship $n_i = X_i n_T$, where X_i is the volume fraction of the i^{th} diatomic species. The number densities of the vibrational levels of species i are evaluated by assuming that these levels are in Boltzmann equilibrium at the local static temperature, i.e.

$$n_{i,v} = X_i n_T \frac{e^{E_{i,v}/T}}{\sum_{w=0}^{Vmax} e^{-E_{i,w}/T}}$$

It has been found that this assumption does not affect the solution downstream [12].

At the exit plane, all the components of velocity, and temperature are evaluated using setting their second derivative to zero in the axial direction. The species number densities and the mass density are evaluated in a similar manner, i.e. by setting their second derivatives to zero, if the flow is supersonic. In case the flow is subsonic at a point on the exit plane, the ideal gas relationship ($P = n_T k T$) for temperature and total number density is used to determine the mass density ($\rho = \sum_{i=1}^{i=N} m_i n_i$) based on a specified value of the static pressure. This equals the value of static pressure at

a point on the exit plane with Mach number closest to one and is updated every time-step. This is done to avoid discontinuities in the pressure profile at the exit-plane that would otherwise occur due to a switch in the boundary condition for mass-density. All number densities (except one) are evaluated by setting their second derivatives to zero in the axial direction. The remaining number density is evaluated by using the algebraic relationship between mass density and total number density.

At solid walls, the all species number densities are evaluated by setting their second derivatives in the radial direction to zero. The mass density on solid walls is also evaluated in a similar manner. This is justifiable as processes occurring on the scale of sheath thicknesses (Debye length) are not considered. Another merit of this boundary condition is that it has proved to most stable numerically. On the cathode, temperature is evaluated by setting its second derivative to zero in the radial direction. This is different from other works [34, 36, 37, 41] where a temperature distribution is prescribed on the cathode surface with the maximum temperature at the cathode tip. This prescription leads to discontinuities at the cathode tip where the temperature changes by about 20,000-30,000 degrees K over length scales smaller than a millimeter. This leads to numerical difficulties. In view of the fact that the cathode tip is hot enough to melt, such a boundary condition on temperature is not entirely unrealistic. On the anode surface, the temperature is maintained at a fixed value. Setting the second derivative of temperature to zero radially yields runaway temperatures, and hence not used. No-slip conditions are specified on all solid surfaces. Thus, all the velocity components are set to zero at the cathode and anode surfaces. Symmetry conditions are imposed on the centerline for all variables of interest (except the radial

and swirl component of velocity which are set to zero). Mathematically, this is written as $\partial\phi/\partial r|_{r=0}$, where ϕ represents any dependent variable.

In addition to the above boundary conditions, it is necessary to specify boundary conditions for the magnetic transport equation describing the B-field (B_θ). The B-field is not computed over the entire computational domain. It extends from the axial location corresponding to the cathode tip to the axial location corresponding to the exit plane. Along the radial plane adjacent to the cathode tip, the radial current density is set to 0, i.e. $j_r = 0$, which is equivalent to $\partial B_\theta/\partial x = 0$. B_θ is set to zero along the centerline and at the exit plane of the constrictor. $B_\theta = 0$ is tantamount to imposing symmetry conditions on the magnetic induction at the centerline, while $B_\theta = 0$ at the exit plane prevents the arc from blowing out of the thruster.

The anode is assumed to be a perfect conductor beyond a point on the electrode downstream of the cathode tip, so that the current streamlines enter its surface normally. This is imposed by setting $(\vec{\nabla} \times \vec{B}) \cdot \vec{s} = 0$, where $\vec{s}$ is the unit tangent vector along the anode surface. This formulation allows current lines to attach anywhere on the anode surface downstream of the prescribed attachment point. Such a formulation is required since the phenomena governing breakdown (i.e. initiation of the arc) and extinction of the arc are not modeled. At a given power level, more than one combination of attachment point and conductivity floor (σ_{floor}) results in a stable solution. Points on the anode surface upstream of the prescribed attachment point have a prescribed B_θ profile based on the total current, i.e. $B_\theta = \mu_o I / 2\pi r$. This approach used to model the attachment point has a more rational basis. Unlike the approach used by Miller et.al [37], the attachment point is not dictated by numerical stability, nor does our formulation require a current distribution to be imposed on

Figure 5.2: Schematic of the 1 KW Arcjet describing Boundary conditions

the electrodes as done by Rhodes et.al [36]. The distinguishing feature of the model used in describing the arc phenomena in this work is that it does not have any ad hoc adjustable parameters as reported in some other simulations [36, 37, 38, 39]. The boundary conditions described above are summarized in Tables 5.1 and 5.2 (See figure 5.2).

(C' is any prescribed attachment point on the anode between B and C)

Initial Conditions

The wave-like nature of the left hand side of the governing equations make it necessary to prescribe appropriate initial conditions to obtain a converged solution. The radial velocity, u , is set to zero everywhere. Figure 5.3 shows the variation of axial velocity along three radial locations. Figure 5.4 shows the initial variation of static

	ABCD (Anode)	DE (Exit Plane)	EF (Centerline)	FGH (Cathode)	HA (Inlet)
ρ	$\partial^2 \rho / \partial r^2 = 0$	$\partial^2 \rho / \partial x^2 = 0$ or from P_{exit}	$\partial \rho / \partial r = 0$	$\partial^2 \rho / \partial r^2 = 0$	Equation of state
u	$= 0$	$\partial^2 u / \partial x^2 = 0$	$= 0$	$= 0$	$u = 0$
w	$= 0$	$\partial^2 w / \partial x^2 = 0$	$\partial w / \partial r = 0$	$= 0$	$\partial^2 w / \partial x^2 = 0$
T	Prescribed	$\partial^2 T / \partial x^2 = 0$	$\partial T / \partial r = 0$	$\partial^2 T / \partial r^2 = 0$	from T_o
n_e	$\partial^2 n_e / \partial r^2 = 0$	$\partial^2 n_e / \partial x^2 = 0$	$\partial n_e / \partial r = 0$	$\partial^2 n_e / \partial r^2 = 0$	$\partial^2 n_e / \partial x^2 = 0$
n_H	$\partial^2 n_H / \partial r^2 = 0$	$\partial^2 n_H / \partial x^2 = 0$	$\partial n_H / \partial r = 0$	$\partial^2 n_H / \partial r^2 = 0$	$\partial^2 n_H / \partial x^2 = 0$

Table 5.1: Boundary conditions for flow variables

	BC'	C'D	DE	EF	BF
B_θ	Prescribed	$\vec{j} \cdot \vec{t} = 0$	$B_\theta = 0$	$B_\theta = 0$	$j_r = 0$

Table 5.2: Boundary conditions for electromagnetics

temperature. The initial static temperature is such that the temperature is increased linearly from a prescribed inlet static temperature to a prescribed temperature at the constrictor. This temperature is held fixed till the end of the constrictor and then decreased linearly to a prescribed value at the exit plane. Figure 5.5 depicts the initial variation of static pressure in the arcjet. A pressure distribution is prescribed axially. The pressure is maintained at a constant value (Stagnation Pressure), till the beginning of the converging portion and then reduced linearly to a low value up to the exit of the constrictor. The pressure is maintained constant at this low value from the exit of the constrictor to the exit plane of the thruster. The prescribed value of the static pressure downstream of the constrictor is usually a very small number chosen to represent near vacuum conditions. The number densities of all the species are

Figure 5.3: Initial Velocity Profiles

given a constant value or specified distributions. Figures 5.6 and 5.7 show the initial variation of molecular hydrogen and electron number densities. Knowing the number densities, the temperature, and the pressure at each axial location, the mass density is obtained. The magnetic transport equation does not require any initial guess as it is an elliptic equation. However, the presence of the electrical conductivity (σ) in the magnetic transport equation, indirectly, requires reasonable initial profiles to be prescribed for the temperature and number densities. The converged solutions are not influenced by the actual values of the dependent variables, in the initial distributions however, reasonable profiles are required for the simulations to time-march in a stable manner.

Figure 5.4: Initial Temperature Profiles

As mentioned in Chapter III, in addition to reasonable initial profiles, addition of artificial dissipation to the governing equations is essential for time-marching the system of equations to convergence. The artificial dissipation term used in the modeling of arcjets is as follows:

$$\mu_x \frac{\partial^2 \phi}{\partial x^2} + \mu_r \frac{\partial^2 \phi}{\partial r^2}$$

where ϕ is any dependent variable. The dissipation term is also treated implicitly.

The form of μ_x and μ_r is problem-dependent. For the 1 KW arcjet, algebraic forms for μ_x and μ_r used were as, $\mu_x = \rho * w * dx/2$, $\mu_r = \rho * dr/2$, where dx and dr denote mesh-spacing in the axial and radial directions. This model was used for all

Figure 5.5: Initial Pressure Profile

equations other than the axial momentum equation. The term describing artificial dissipation in the axial momentum equation is given by:

$$\mu_{x3} \frac{\partial^2 w}{\partial x^2} + \mu_{r3} \frac{\partial^2 w}{\partial r^2}$$

where

$\mu_{x3} = \rho * w * dx / 8$ and $\mu_{r3} = \rho * dr / 8$. The forms of μ_r and μ_x are proportional to the cell Reynolds number. The constant coefficient multiplying these terms allows one to vary the amount of dissipation. The specific form of μ_r and μ_x were determined by trial and error. The set of governing equations along with the boundary and initial conditions and the form of the artificial dissipation needed for stable time-marching

Figure 5.6: Initial Molecular Hydrogen Concentration Profiles

described above, completes the formulation of the problem. This formulation can be used to study flows through arcjet thrusters with different geometries and operating conditions. An independent grid generation routine computes physical dimensions of the geometry under consideration and the transformation derivatives as explained in Chapter III.

Simulations can be performed for a given value of current, power level and mass-flow rate. This allows a direct comparison of numerical results with experimental data under similar operating conditions. The operating current is specified and mass-flow rate can be varied by means of the prescribed value of the total pressure (P_o). The

Figure 5.7: Initial Electron Concentration Profiles

required power-level (as measured by a product of Voltage and Current in the experiments) is obtained by computing $\int_V \vec{E} \bullet \vec{j} dV$, where V represents the volume of the flow domain. This method of evaluating the total power is consistent with Poynting's Theorem [6]. The power-level can be varied by the value of the “conductivity floor” used in the simulations. Since the mass-flow rate and the power-level have to be determined a posteriori, the values of the floor and the upstream total pressure are adjusted in concert until the converged solutions yield the desired power level and the mass-flow rate. Since the power-level is decided on the basis of the “conductivity floor”, this is not an ad-hoc adjustable parameter and remains fixed for a given set of

Figure 5.8: 1 KW Arcjet Geometry (all dimensions in mm)

operating conditions, namely, power-level, current and mass-flow rate. This formulation thus does not have any adjustable parameters which can be varied in an ad-hoc manner.

5.3.4 Case-study:- 1 KW Arcjet Geometry

Based on the formulation discussed above, flow through two different arcjet thrusters have been modeled, namely a 30 KW arcjet thruster [26] and a 1 KW arcjet thruster with hydrogen as the propellant. Unfortunately, there do not exist detailed experimental results for the 30 KW arcjet geometry. However, experimental measurements have been performed by groups at Phillips Laboratory - Edwards Air Force Base [42] and Stanford University [43, 44] on 1 KW arcjet thrusters (see Figure 5.8) with H_2 as the propellant. The operating conditions for these experiments were at a power level ≈ 1.4 KW, current ≈ 10 Amps and a mass-flow rate of ≈ 13 mg/s. Simulations for the aforementioned experimental conditions (geometry, propellant and operating

Figure 5.9: Physical Domain of the thruster with grids showing half of the channel

conditions) were performed in order to compare results of the simulations directly with those obtained from experiments. In this subsection, comparison of the results of the numerical simulation with experimental data is discussed. Additionally, flow characteristics of interest obtained from the simulations for which no experimental data exist are also presented and discussed.

The 1 KW arcjet geometry shown in figure 5.8 was discretized using a 150×50 grid. Figure 5.9 shows the physical domain with the grids. For the sake of clarity only every 10^{th} grid in the axial direction and 4^{th} grid in the radial direction have been shown. This grid size was chosen on the basis of a grid convergence study performed on a 30 KW arcjet geometry. The maximum discrepancy between the converged results for a coarse grid (60×50) and a fine grid (120×50) in the case of a 30 KW geometry was less than 0.1 %. The 1 KW arcjet geometry has a smaller length and a more severe exit-to-throat area-ratio (225) as compared to the 30 KW arcjet geometry (25), and hence a much finer grid was chosen to adequately resolve the gradients. All

the simulations were performed in uni-processor mode on the CRAY Y-MP at the Ohio Supercomputer Center. Speeds on the order of 180-200 Mflops were obtained.

The plasma in the Hydrogen arcjet is assumed to comprise of molecular hydrogen (H_2), atomic hydrogen (H), electrons (e^-), and singly-ionized hydrogen atoms (H^+). H_2 is the only diatomic species. No vibrational states of molecular hydrogen are considered and a single temperature is used to describe the heavy particles and the electrons. Quasi-neutrality is assumed, which allows us to set the number density of e^- equal to that of H^+ . The net rate of production/depletion of a given specie (i.e. the source term $\dot{n}_m$ in the monatomic species equation) is evaluated from the specific chemical processes modeled. The following four processes are considered in the present study.

It must be pointed out that the present formulation does not preclude the inclusion of more species. The forward rate constants for the first two reactions (i.e. 5.1 and 5.2) are given in [45], while those for the next two (i.e. 5.3 and 5.4) are given in [46]. The reverse rate constants are then computed from the forward rate constants and the respective equilibrium constants based on partition functions [17]. The rate constants are treated explicitly while the number densities multiplying them are treated implicitly in the differencing procedure.

Case	P_o	σ_{floor}
Upstream	2.65e5 N/m ²	5.25 mho/m
Downstream	2.85e5 N/m ²	23 mho/m

Table 5.3: Operating Conditions for the two arc attachment cases

The dimensions of the constrictor in the 1 KW arcjet geometry are extremely small (see Figure 5.8). The constrictor diameter is 0.635 mm while its length is about 0.381 mm. Since the location of the arc attachment is not precisely known, simulations were performed for two different arc attachments - upstream attachment and downstream attachment. It is assumed that the arc attaches itself anywhere downstream of the prescribed attachment point. *In the upstream attachment case*, the prescribed attachment point is a point on the anode closest to the cathode tip, whereas in the *downstream attachment case* it is at the end of the constrictor. The axial distance from the cathode tip to the attachment point corresponds to 0.508 mm for the upstream attachment case and 1.651 mm for the downstream attachment case. The intent of this comparative study is to elucidate the importance of arc attachment on energy loading of the propellant stream. The solutions obtained from these two simulations are compared against two sets of experimental results. These two cases (i.e. upstream attachment and downstream attachment case) differed in the total stagnation pressure and conductivity floor, but were identical in total current, power-level and mass-flow rate. The operating conditions for these two arc attachment cases are given below. The total upstream pressure and the σ_{floor} had to be adjusted in concert so as to obtain nearly the same mass-flow rate and power in the upstream and downstream attachment cases. Convergence was judged on the basis of percentage

Figure 5.10: Calculated current contours showing the upstream attachment case

variation of total power and mass-flow rate over 10000 time-step intervals. When fluctuations in mass-flow rate and power level were within 2% of the desired values the solution was assumed to have converged. This approach had to be adopted as changes in the stagnation pressure or σ_{floor} bring about ripples in the computational domain. It is imprudent to expend large amounts of CPU time to allow these oscillations to die down as their impact on the final solution is negligible. Moreover, the experimental data with which the results of the simulation are compared against have errors of about 10-25%.

Converged results obtained based on considerations discussed above are compared with experimental data. The similarities and differences between experimental data and the results of the present work are discussed next.

5.3.5 Results and Discussion

Figures 5.10 and 5.11 show calculated enclosed current contours for the upstream

Figure 5.11: Calculated current contours showing the downstream attachment case

and downstream attachment case, respectively. As explained in the previous section, in the downstream attachment case, the arc is free to attach itself anywhere downstream of the point on the exit of the constrictor (on the anode) and in the upstream attachment case, the arc is free to attach itself anywhere downstream of the point on the anode that is closest to the cathode tip. The current contours shown reflect the prescribed attachments. Figures 5.12 through 5.15 show comparisons between the results of our simulation for the upstream and downstream attachment case with experimental measurements from [42, 43, 44] along the exit plane. Figure 5.12 shows that the H-atom number density along the exit plane predicted by the upstream attachment case matches the experimental data very well, however there is a noticeable difference in the experimentally obtained H-atom concentration and those predicted by the model (downstream attachment case) near the centerline. Both the upstream and downstream attachment cases match the experimental data very well close to the wall. It is seen that the downstream attachment case has a pronounced bulge whereas

Figure 5.12: Comparison of the predicted hydrogen atom concentration at the exit plane with experimental data. Circles - H-atom concentration obtained by LIF measurements on H-atoms from [42]; Solid line - downstream attachment case; Solid line with asterisks - upstream attachment case.

the upstream attachment has a mild but noticeable bulge. This can be explained on the basis of the temperature profiles and molecular hydrogen concentrations (see figures 5.14 and 5.15). The bulge is primarily due to the opposing effects of a radially increasing H_2 number density (which tends to increase the rate of formation of H-atoms) and a radially decreasing temperature (which tends to decrease the rate of formation of H-atoms). The increasing H_2 number density causes an increase in the local rate of dissociation whereas the decreasing temperature decreases the reaction rate constant responsible for the dissociation. These opposing effects produce a local

Figure 5.13: Comparison of calculated radial distribution of streamwise velocity at the exit plane with experimental data. Solid curve - downstream attachment; Solid curve connected by asterisks - upstream attachment; circles - experimental data from [42]; '+' - experimental data from [47].

maximum in the H-atom concentration away from the centerline and the boundary as well. The temperature drops more steeply in the downstream attachment case as compared to the upstream attachment case which explains the more pronounced bulge in the downstream attachment case versus the upstream attachment case.

Figure 5.13 shows a comparison of exit-plane velocities for the two cases studied in the present work against experimental data [42]. It can be seen that the agreement is very good in both cases. The upstream attachment case underpredicts the experimentally observed values along the centerline by about 10%. This shows that

Figure 5.14: Comparison of calculated radial distribution of temperature at the exit plane with experimental data. Solid curve - Downstream attachment case; Solid curve connected by asterisks - upstream attachment case; 'o' - experimental data based on LIF measurements on H-atoms from [42]; 'x' - temperature based on uncorrected H-atom LIF data from [43]; '*' - temperature based on Stark corrected H-atom LIF data from [43]; '+' , H-atom emission data from [43]; circle with '+' connected by lines - H_2 Raman spectroscopy data from [43].

the arc attachment does not greatly influence the predicted exit plane velocity profiles. It must be pointed out that other single temperature models also under predict velocities at the exit plane [48, 47].

Figure 5.14 shows the radial temperature profile at the exit plane along with experimental results from [42, 43, 44]. The radial temperature profiles along the exit plane show a marked quantitative difference for the two cases of attachment studied,

though qualitatively, the variations show strong similarities. The noticeable bulge in the temperature profiles is reminiscent of hypersonic thermal boundary layers near cooled surfaces [49]. The cause of the local maximum in the radial temperature profile is due to the opposing effects of viscous dissipation heating the flow and the relatively colder wall trying to cool it. It can be seen that temperatures predicted by the downstream attachment case, compare well with the LIF data reported by [43], whereas the upstream attachment case predicts temperatures close to those reported by [42]. The scatter in the experimental data makes it difficult to ascertain the presence or absence of bulges in temperature. It is also instructive to note that the temperature measurements made by Storm et. al [43] differs considerably from those reported by Wysong et. al [42], even though the measurements have been made for two arcjets supposedly operating under identical conditions. Temperature inferred on the basis of H_2 Raman spectroscopy differs from temperature measurements made by LIF [43] on H-atoms. The reason for the difference in the LIF temperature measurements reported by [42] and [43] could well be due to different arc attachments in the two experiments. The difference in exit-plane temperature measurements made on the basis of LIF and H_2 Raman spectroscopy as reported by [43, 44] could well be due to non-equilibrium effects. Direct Simulation Monte Carlo (DSMC) calculations by Boyd [48] show that there exists a considerable dis-equilibrium between the internal and external (translational) modes of H_2 molecules at the exit plane. These calculations show centerline vibrational temperatures at the exit plane close to 3000 K, centerline rotational temperatures near 2000 K, and the centerline translational temperatures about 1000 K. These differences between the internal modes and external mode temperatures could well be explained by dis-equilibrium between the internal

and external modes of molecular hydrogen. Due to the high velocities and low densities at the exit plane, the finite rates for V-V, V-R, and V-T transfer could lead to this dis-equilibrium. Further, it is well known that V-T rates increase with vibrational quantum number so that the translational temperatures obtained in the experiments using LIF on the H-atom may be inferring the vibrational temperatures of excited H_2 molecules via

where H^* is translationally hot. Thus V-T relaxation of higher vibrational levels of H_2 by H could result in the translational temperatures of H-atoms being higher than that of molecular hydrogen.

Figure 5.15 shows a comparison between the molecular hydrogen concentration at the exit plane for the two cases of arc attachments studied in the present work with measurements reported in ref [48]. The downstream attachment case shows wiggles in regions close to the centerline. This is lack of sufficient dissipation in regions close to the exit plane in the downstream attachment case. It can be seen that the profiles for the two cases of arc attachment are quantitatively markedly different near the centerline. However, the profiles are similar in shape. It is seen that the upstream attachment case over-predicts the concentration of molecular hydrogen by a factor of 2, whereas the downstream attachment is closer to the experimentally reported values near the centerline. This is expected since the mass-flow rate is very nearly the same for the experiment and the two cases studied, and an under-prediction of velocity would be consistent with an over-prediction of mass density and hence molecular hydrogen concentration (n_{H_2}). The bulge in the n_{H_2} follows the variation in temperature. A reduction in the temperature with increasing distance from the

Figure 5.15: Comparison of radial distribution of molecular hydrogen concentration at the exit plane with experimental data. Solid curve - downstream attachment; Solid curve with asterisk - upstream attachment; '+' H_2 Raman spectroscopic data from[43].

centerline assists recombination of atomic hydrogen to molecular hydrogen. The slight increase in temperature brings about a reduction in n_{H_2} . In the subsonic region, close to the wall, the pressure is held constant so that the steep drop in temperature results in an increase in n_{H_2} .

Figure 5.16 shows the variation of electron concentration at the exit plane for the two arc attachment cases studied and experimental data reported in [43]. The upstream attachment case (denoted by asterisks) underpredicts the electron concentration by about two orders of magnitude whereas the downstream attachment (solid

Figure 5.16: Comparison of radial distribution of electron concentration at the exit plane with experimental data. Solid line - downstream attachment; solid line with asterisks - upstream attachment; '+' experimental data from [43].

curve) compares very well with experimental data (denoted by '+'). This is clearly due to the magnitudes of the temperatures for the two attachment cases (see Figure 5.14). Further the maximum temperature (see Figure 5.20) near the constrictor is greater for the downstream attachment case. This, coupled with the fact that the downstream attachment case has a higher velocity tends to preserve the “memory” of the high electron concentration values from the constrictor manifesting in higher values at the exit plane. This explanation is consistent with the temperature and electron concentration along the centerline shown in figures 5.20 and 5.22.

Figure 5.17: Percent dissociation fraction at the exit plane.

Figure 5.17 shows a variation of the dissociation fraction along the exit plane. As explained earlier, the wiggles in the downstream attachment case close to the walls is due to the lack of sufficient artificial dissipation. It is seen that the dissociation fraction is considerably high - close to 30%. This high value of dissociation fraction is an indication of the frozen flow losses. Ideally, the gas stream exiting the thruster should consist of unexcited molecular hydrogen only, which would mean that no electrical energy is lost in internal modes or to processes such as dissociation and ionization.

Figure 5.18 shows the predicted pressures along the exit plane for the two arc attachment cases under consideration along with experimental data from [50]. The

Figure 5.18: Comparison of radial distribution of static pressure at the exit plane with experimental data. Solid line with circles - downstream attachment; Solid lines with asterisks - upstream attachment case; circles - experimental data from[50].

downstream attachment case shows wiggles in regions close to the centerline. This is due to insufficient artificial dissipation which introduces wiggles in the total number density, which in turn introduces wiggles in the exit plane pressure profiles. It is seen that both the upstream and downstream attachment cases qualitatively agree well with experimental data. In regions close to the centerline, the variation in static pressure is negligible, both in the experiment and the present work. However, the pressure begins to drop off steeply after this initial flat portion near the centerline. It

Figure 5.19: Comparison of centerline axial velocity with experimental data. Solid line - downstream attachment; solid line with asterisks - upstream attachment; '+' experimental data from [44].

is further seen that static pressure along the exit plane is not constant in the supersonic region and the bell-shaped profile is due to the combined effects of increasing total number density (n_T) and decreasing temperature. It is also possible that the region near the centerline is nearly isentropic and hence the static pressure is constant whereas it drops in regions away from the centerline due to viscous boundary layer effects. It is interesting to note that static pressure values based on the numerical results of Butler et. al [50] agree quantitatively with those predicted by the downstream attachment case.

Figure 5.19 shows a comparison of the axial variation of the streamwise component of velocity along the centerline. Also shown are experimental measurements from [44]. The solid curve represents the downstream attachment case whereas the asterisks denote the upstream attachment case. Experimental data is denoted by the '+' signs. Figure 5.19 shows considerable discrepancy qualitatively between the results of this simulation and those reported experimentally in the region close to the exit of the constrictor. It is seen that the agreement is better in regions closer to the exit plane and the experimentally reported velocities are bounded by the two different attachment cases. It is important to point out the fact that the experimental axial velocity profile shows two distinct slopes. A steep gradient is observed near the exit of the constrictor which is followed by a much more gradual slope in regions away from the constrictor. The authors of [44] report that the three data points closest to the constrictor contain the largest experimental error. They attribute this error to the luminosity associated with this region on account of its proximity to the arc. However, the steep drop in velocity at the exit of the constrictor observed experimentally appears to be indeed real. In regions close to the exit of the constrictor, the flow is supersonic and addition of heat due to the arc can bring about its rapid deceleration. The effect of increasing area on the other hand, tends to keep the flow supersonic. This appears to be the best evidence showing that the arc attachment in the experiments of Cappelli et.al [44] is indeed downstream of the constrictor on the anode. Heat addition due to the arc ceases after a short distance from the exit of the constrictor. In this region, the flow slows down due to viscous effects. This phenomena is primarily responsible for the presence of two distinct slopes in the centerline velocity profile reported experimentally. This salient feature of the axial

velocity profile evident in the experimental profile is not captured by the present simulation largely due to the model of the arc. The constriction of the arc is not modeled well enough in this work, especially in the upstream attachment case. The downstream attachment case, however, “forces” the arc to attach downstream of the constrictor. This forced attachment is responsible for some constriction of the arc. Consequently, the centerline velocity profile in the downstream attachment case, does exhibit a steeper gradient in velocity near the exit of the constrictor as compared to regions further away. However, the upstream attachment case shows no such inflection. The peak axial velocity predicted by the downstream attachment case also agrees quantitatively with experiments. In addition to the lack of constriction of the arc, the effects of artificial dissipation are also highest in regions near the constrictor. These two reasons could be principally responsible for the large discrepancy between experiment and simulation in centerline velocities close to the constrictor.

Figure 5.20 shows the centerline variation of temperature for the two arc attachments studied along with experimental data reported in [48]. The solid curve represents the downstream attachment case, whereas the asterisks denote the upstream attachment case. Experimental data is represented by '+'. These experimentally measured temperatures have not been corrected for Stark broadening and hence are expected to over-predict the real temperatures. Nevertheless the two arc attachment cases studied predict values which are in reasonable agreement with each other. A noteworthy feature is that the downstream attachment case predicts a peak temperature which is almost 10,000 K above that predicted for the upstream attachment case. The jaggedness in the temperature profile is again due to the effects of artificial dissipation. The location of the temperature maximum can also be seen to be further

Figure 5.20: Comparison of centerline temperature with experimental data. Solid line - downstream attachment; solid line with asterisks - upstream attachment; '+' experimental data from[44].

downstream in the downstream attachment case as compared to the upstream attachment case. This has important consequences for energy loading of the propellant stream. The higher predicted temperature and the location of the maximum temperature explain the higher electron concentration and temperature at the exit plane of the thruster. This figure clearly indicates the importance of arc attachment and its effect on the exit plane profiles.

A detailed comparison between the results of this work and experimental data from two different groups along the exit plane and the centerline highlights the strengths

Figure 5.21: Profiles of calculated centerline hydrogen atom concentration. Solid lines with circles - downstream attachment; solid lines with asterisks upstream attachment.

and weaknesses of our model. In addition to the above comparisons, the axial variation of parameters of interest such as atomic hydrogen concentration, electron concentration and molecular hydrogen concentration are presented. Though experimental data are not available for these quantities, it is nonetheless important to assess impact of the energy loading on these quantities. In all these profiles, the solid curve with asterisks denotes the upstream attachment case, whereas the solid curve joined by circles denote the downstream attachment case.

Figure 5.21 shows the axial variation of atomic hydrogen along the centerline. It is seen that the H-atom concentration tracks the temperature variation. Near the

Figure 5.22: Profiles of calculated centerline electron concentration. Solid lines with circles - downstream attachment; solid lines with asterisks upstream attachment.

constrictor, where there is maximum energy addition, the concentration of H-atoms is maximum. However, as the flow exits the high temperature region, the concentration of H-atoms drops due to recombination at lower temperatures. Figure 5.22 shows the variation of electron concentration along the centerline. The variation of electron number density is also akin to the H-atom variation, in that it tracks temperature. Figure 5.23 shows the variation of molecular hydrogen concentration along the centerline. It can be seen that the number density of molecular hydrogen (n_{H_2}) drops significantly in the region close to the constrictor. This is due to the presence of the arc which brings about dissociation of hydrogen molecules. However, n_{H_2} increases

Figure 5.23: Profiles of centerline molecular hydrogen concentration. Solid lines with circles - downstream attachment; solid lines with asterisks upstream attachment.

in the relatively colder diverging section of the arcjet due to recombination. It is observed that the concentration of H_2 is less in the diverging section versus the plenum. This is primarily due to the pressure drop that is encountered in the diverging section. In all figures that depict centerline variation of quantities, there is a considerable amount of jaggedness in regions close to the constrictor. This is primarily due to the large gradients in that region and the effects of artificial dissipation.

The discussion thus far has examined the profiles of temperature, velocity and species concentration along the centerline and the exit plane. The results have been

compared and contrasted with experiments where possible. It is instructive to examine the plausible causes of disparity between experimental results and the results of this work.

The discrepancies in predicted values and those obtained experimentally could be due to two main reasons - physical model describing the complex energy transfer mechanism from the arc to the propellant and shortcomings in the numerical scheme used. A single temperature description of the plasma and the modeling of the arc itself could be two main physical reasons. A single temperature continuum model is not strictly applicable in the low density regions characterizing the diverging section of the arcjet, where the effects of non-equilibrium are most likely to be acute as pointed out earlier. The electromagnetics model in this work is unable to capture the constriction of the arc correctly. During the actual operation of the arcjet, the arc emanates from regions close to the cathode tip and attaches itself on the anode. It is believed that this attachment in the experiments is at a point slightly downstream of the constrictor. Since the exact extent of the region on the cathode from which the arc emanates is unknown, the electromagnetic calculations in this work begin at the cathode tip and $j_r = 0$ is applied along the plane corresponding to the axial location of the cathode tip. Such a prescription gives rise to a diffuse arc. This deficiency in the modeling of the arc is most likely to impact the energy loading of the propellant stream and hence affect predictions of velocity, temperature and species concentrations. Physical models describing the variation of transport properties such as viscosity, thermal conductivity, and reaction rates also play an important role in the determination of the velocity, temperature and species concentrations in the arcjet. The transport properties are evaluated at present using the mean-free-path

theory and could be in error by a factor of two or three [9], which could influence the results of the numerical simulation.

Time-discretization of the governing equations gives rise to numerical dissipation in most numerical schemes. The LBI scheme used in this work, requires the addition of artificial dissipation to time-march in a stable manner. Ideally, minimum dissipation required for overall stability of the system of equations should be added. However, this is very difficult to do. Empirical models for artificial dissipation based on flow variables, can lead to addition of large amounts of dissipation in certain regions in the physical domain. The addition of dissipation affects the accuracy of the results in supersonic flows. The artificial dissipation model used in this work, results in the artificial dissipation being highest in the constrictor region. Based on the expression for the dissipation model discussed earlier, in the plenum where the gas is cold, mass density is high but the flow is slowly moving and hence the term μ_x is low. In the supersonic region far from the constrictor, axial velocity is high but the mass density is very low which leads to a lower value of artificial dissipation. However, in the constrictor region, the flow is accelerated due the arc, but the density is still high, consequently the dissipation is highest in this region due to a high value of μ_x . Since the energy transfer from the arc to the propellant takes place in the constrictor region, the energy loading of the propellant stream is bound to be influenced by the effects of numerical dissipation. A parametric study is perhaps the best way of studying the effect of dissipation on the accuracy of the solution. In Chapter IV it was shown that artificial dissipation affects the accuracy of the solution. Quasi 1-D simulation on a geometry similar to the 1 KW arcjet thruster (which has a severe exit-to-throat area ratio of 225) show that artificial dissipation affects the

accuracy of the solution by about 10% for 150 grid points in the axial direction (see Chapter IV). Additionally, it was inferred in Chapter IV, that increasing the number of grid points in the computational domain led to a reduction in the effects of dissipation on the overall accuracy of the solution. Since the effects of dissipation are unknown a priori, simulations in this work were performed for a reasonably fine grid after which the effects of dissipation were examined upon convergence. To study the influence of artificial dissipation, the term μ_3 was reduced by a factor of 4. To obtain similar mass-flow rate, the stagnation pressure had to be reduced by about 5%. The qualitative shapes of the dependent variable did not change. The values of the dependent variables changed by less than 5%. Such a study, though not extensive, serves to show that the effects of dissipation do affect the accuracy of the solution however within acceptable limits.

The above discussion underscores several important issues in the experimental and numerical investigation of arcjets. A comparison of experimental results from two different groups (at Phillips Laboratory - Edwards Air Force Base and Stanford University) for a 1 KW arcjet geometry supposedly operating under identical conditions are considerably different. Though it is believed that the arc attaches just downstream of the constrictor on the anode, there could well be differences in the actual location of the attachment of the arc in these two experiments. The scatter in the experimental data reported in [42] gives credence to the theory that there may be minute changes in the attachment of the arc during different runs. The uncertainties associated with experimental data make it difficult to infer the shapes of profiles of measured quantities unambiguously. The results of this simulation have shown that moving the prescribed attachment point by a distance of about 1 mm greatly impacts

the solution. Thus both the experimental data and the results of this simulation highlight the importance of energy loading of the propellant stream by the arc and its effects on the flow variables in the arcjet thruster and at the exit-plane.

Comparison of this work with experimental data brings to fore the strengths and weakness of this model. The model not only predicts trends correctly, but also the quantitative agreement of the overall solution with experiment is very good. These results can be obtained in a reasonable amount of CPU time on the CRAY Y-MP (a typical simulation requires less than 10 hours of CPU time). Most importantly, there are no adjustable parameters in this simulation. However, the physical model does suffer from two main deficiencies which are ultimately removable. A single temperature description of the plasma is unrealistic, especially in regions near the exit plane. DSMC simulations by Boyd [48] show a marked degree of dis-equilibrium between the various internal modes and translational mode for molecular hydrogen. The model used in this work does not address state-specific kinetics and hence is unable to capture this dis-equilibrium. Constriction of the arc is not predicted well by the present model. From the perspective of modeling, the upstream attachment case is less constraining as the arc is allowed to attach at any point downstream of the prescribed attachment point and this case gives better agreement with experimental data. However, this contradicts experimental observation of the location of arc attachment. It appears that the upstream attachment case is able to mimic the energy loading of the propellant stream better than the downstream attachment case. Although numerical dissipation is a likely source of error in the constrictor region, the accuracy of the overall solution (especially in regions far from the exit of the constrictor) does not appear to be significantly affected. This observation is confirmed by the fact that

maximum discrepancy between simulation and experiment exist in regions close to the constrictor whereas it is much less in regions near the exit plane. Improvements in the electromagnetics model and modification of the dissipation term to minimize dissipation in the constrictor regions are the two most important changes that need to be made to the current single temperature model.

The next section discusses the study of high pressure arcs encountered plasma torches.

5.4 Case Study II: Variable Polarity Plasma Arc (VPPA) Welding

5.4.1 Introduction

Electric arcs are used widely in applications ranging from industrial-scale arc furnaces and switchgears, to materials synthesis and processing. Plasma torches form an important class of electric arcs. Plasma torches are used as clean and efficient sources of intense heat in many industrial applications. Plasma spray coating and welding are two notable examples. Welding is one of the basic industrial processes used widely in manufacturing and fabrication of parts and components. Study of techniques to produce joints of high quality and strength are thus of great importance. Consequently, a great deal of effort has been expended in recent years to determine the characteristics of electric arcs. This second case study involves just such a welding arc.

Electric arc-welding processes consist of an electrode and a workpiece of opposite polarities. An arc is struck by applying an electric field between two electrodes, causing current flow through the partially ionized gas column (established between the electrodes). The heat generated in the arc produces the high temperatures needed to

sustain the gas in its ionized state. The thermal energy is transferred to the workpiece primarily due to particle fluxes [51] causing it to melt; the subsequent solidification of this molten region, termed the weld pool, forms the weldment or actual joint. Gas-Tungsten Arc Welding (GTAW), Gas-Metal Arc Welding (GMAW) and Variable Polarity Plasma Arc (VPPA) welding are some of the popular methods of welding. In many cases, a discharge is initially struck between an electrode and another auxiliary electrode using high frequency AC excitation. Then the main arc is struck between the electrode and workpiece by transferring the discharge. Such an arc is called a transferred arc.

The underlying difference between the VPPA technique (Plasma Arc Welding) and the GTAW (and GMAW) is that *the VPPA torch has a continuous forced flow of plasma gas* whereas the GTAW and the GMAW are free-burning arcs. In a free burning arc, any induced flow such as the cathode jet is dominated by the magnetohydrodynamic pumping from the arc itself and not by any forced gas flow. In the plasma arc welding process, the plasma gas flow is constricted by a metallic nozzle around the cathode. The VPPA torch assembly essentially consists of a central electrode concentric with two enclosing outer surfaces which confine the main plasma gas and shield gas flows. These are called the constricting nozzle and the shield gas nozzle, respectively. The constricting nozzle confines the plasma gas and also acts as the anode for supporting a pilot arc (non-transferred arc). The shielding gas flows through the annulus between the constricting nozzle and the shielding gas nozzle. Both the plasma and shield gases are inert. Typically, argon is used as the plasma gas while the shield gas is either argon itself or helium. An inert shielding gas is used to reduce oxidation of the work piece due to entrainment of ambient oxygen.

The main plasma gas enters the torch - cold and at low velocities, and is rapidly accelerated near the exit plane of the torch by Ohmic heating within the arc. The resulting high velocity plasma jet then impinges on the workpiece (transferred arc), and provides enough penetration to produce a deep weld and/or a keyhole.

The plasma arc welding torch can be operated in one of several modes - straight polarity, reverse polarity, or variable polarity. The discharge is initiated by applying a high frequency alternating voltage between the inner electrode (cathode) and the constricting nozzle (anode) so as to establish a pilot arc. The polarity of the pilot arc does not alternate. The nozzle is always held positive with respect to the electrode (by about 20 V). The main arc (transferred arc) is then struck between the workpiece and the cathode. The workpiece is always grounded and the inner electrode is biased positive or negative with respect to the workpiece. This bias voltage is usually around 30 V.

When an arc is struck by applying an electric field between two electrodes, the positive ions and electrons in the arc column act as charge carriers. By virtue of its significantly lower mass, electrons acquire a greater velocity as compared with the ions in the interelectrode space. This fact is made use of in the various modes of operation of the Plasma Arc Welding (PAW) process. In the straight polarity mode, the central electrode acts as the cathode (held negative) and the workpiece acts as the anode. The flux of electrons impinging on the workpiece is much greater than the ion flux impinging on the cathode. Hence, this mode of operation is used when the objective is to deliver a maximum amount of heat to the workpiece with minimal deterioration of the electrode. In the reverse polarity mode, the electrode is positive with respect to the workpiece. This subjects the workpiece to a cleaning process called

“cathodic cleaning”, on account of the surface bombardment by heavy positive ions. This is of importance when the work-piece is Aluminium. In the variable polarity mode, the polarities of the workpiece and the central electrode are reversed at fixed time intervals. This method exploits the merits of both - the straight polarity and the reversed polarity modes of operation. Typically, the torch is operated in the straight polarity mode for about 19 milliseconds and the reverse polarity mode for 4 milliseconds.

The PAW process is gaining popularity over the traditional GTAW process. Some of the advantages of the PAW over the traditional GTAW processes are as follows [52]:

- a) Higher jet velocities as compared to the GTAW process. It has been reported that the velocity of the jet impinging on the workpiece is about four times the velocities attained using GTAW process.
- b) Higher depth of penetration into the weld pool. It is reported in the literature [52] that stagnation pressures of about 25 inches of water (gage) for the plasma gas can bring about a depression of about 4 inches in the weld pool. It is possible to operate the plasma arc in the “keyholing” mode, wherein the plasma jet penetrates the entire workpiece, i.e. the hole through the workpiece opens up in front of the traversing jet and seals up behind it, forming a deep and relatively narrow weld bead. The PAW process thus has the ability to accomplish in a single pass, what requires multiple passes with GTAW.
- c) An open keyhole greatly enhances escape of gaseous contaminants, and on occasions also blows out solid contaminants.

- d) The VPPA welding process exhibits a greater degree of tolerance to contaminants, thereby reducing scrapping.
- e) Welds produced using VPPA are virtually porosity free and require significantly less need for post-process inspection and repair.

The relative merits of the VPPA torch over the GTAW and GMAW has enabled its use in fabricating the external fuel tank of the Space Transport Shuttle (STS) at NASA Marshall Space Flight Center (MSFC) since 1979. Over the years, improvements in the design of the VPPA torch assembly has allowed the extended welding times necessary for completion of lengthy external tank welds, at a current level of hundreds of amperes (typically between 200-300 A). In spite of these improvements, some issues remain to be addressed to enhance future applications. One of the near term goals is to increase the current capacity beyond the present level of 300 A. Another issue of great importance that needs to be resolved is the tendency of the plasma jet to skew or deflect from the axis of the torch. This offsets the weld and creates weld asymmetry, resulting in unacceptable weld bead shapes. Manual or automatic control must be exercised to ensure that the arc is aligned with the weld motion in order to minimize its effects on the weld bead. It has been a subject of speculation that the asymmetry between the central electrode and the orifice (constricting nozzle), either due to initial misalignment or uneven erosion after long hours of operation, is one of the causes. It is also noted that the occurrence of the skew is erratic and random, which leads one to conclude that there may be more than one cause for the occurrence of this skew.

A systematic study of the design and operating conditions of the torch and the plasma jet is required to obtain a better understanding of the operating characteristics

of the torch. The results of such a study would establish plausible links between the skew phenomena, torch design and operating conditions. This should provide a more rational basis for future designs with better performance. With these main objectives in mind the present study endeavored to study flow characteristics in these torches, and the external jets impinging on the work-piece.

5.4.2 Background

A number of groups have attempted to model these plasma jets and compare the results of their computations with available experiments. The experimental results mostly comprise of temperature measurements in the plume of a free jet. The earliest attempts to model plumes of plasma torches [53, 54, 55] required the specification of temperature and velocity profiles at the exit plane of the nozzle as boundary conditions. Lee and Pfender [55] studied the effects of two different temperature and velocity profiles at the nozzle exit on the external flow of a free jet. The profiles chosen were such that the overall mass and energy flow rates in the two cases were identical. In spite of this, the largest temperature difference computed in the external plume domain was 3000 K and the largest velocity difference was 300 m/s. These differences are equivalent to about a 30% variation in temperature and about 100% in velocity. Since these models did not include the arc region within the torch, the temperatures and velocities of the plasma jet at the exit plane of the torch could be obtained only by a gross specification of the mass and energy flow rate. Thus, to obtain realistic information about the flow characteristics in the plume, it is essential to correctly model the arc region in the interior of the torch.

To overcome these deficiencies in the earlier models, Scott et. al [56] attempted to model the torch as a single entity. The region behind the cathode, the arc region and the plasma plume region were all included in the model. This model was a steady, 2-D model which included the swirl component of the flow and a $K - \epsilon$ turbulence model. Further, the plasma and the ambient gas were both argon, so the effects of mixing and entrainment were not included. Westhoff et. al [57] attempted a study similar to that of Scott et. al [56]. However no additional physics was included in their model. Murphy and Kovitya [58] have extended the model of Scott et. al to include the effects of mixing of the plasma gas with an ambient gas. However, these models do not include the effect of shielding gases. They also do not include ionization and recombination reactions, and ionization fractions are computed from equilibrium (Saha) considerations. All the above mentioned models simulate free jets and are thus non-transferred arcs. It is indeed surprising that the above mentioned works are the only models that attempt a numerical solution of the 2-D MHD equations describing plasma arcs. All solve steady equations and do not model transferred arcs.

In contrast to these earlier works, the present work is the *first self-consistent model of transferred plasma arcs*. The governing equations described in Chapter II are solved to obtain the flow characteristics and species concentrations in a *transferred plasma arc*. The internal flow simulations are used to obtain all the flow variables at the exit plane of the torch. The external flow simulation is then used to model the plasma jet impinging on the work-piece by using the exit plane values computed from the internal flow. The flow is assumed to be laminar in the present work. Effects of the shielding gas are included in the external flow simulation. The effects

of ambient entrainment are not included, though the present formulation can be very easily modified to include this effect.

Model validation in the present work is radically different from other earlier and existing investigations. Scott et. al [56] and Murphy et. al [58] have compared the results of their simulations to isotherms obtained experimentally from free jets. Using measured temperature as a measure of model reliability is questionable since the measurement techniques make inherent assumptions about the state of the plasma (such as Local Thermodynamic Equilibrium (LTE)). Fincke et. al [59] discuss the results obtained by two methods - enthalpy probe and laser light scattering experiments. Murphy et. al [58] point out that comparisons reported by Scott et. al [56] are suspect since they used emission spectroscopy to obtain experimental temperature profiles, a technique which relies on the gas being in LTE. On the other hand, the laser light scattering technique for temperature measurement used by Murphy et. al requires a precise knowledge of the gas composition. To avoid these complications, a simple and inexpensive diagnostic technique is used in the present work for model validation. A radial pressure profile is measured on a water-cooled copper plate while the plasma jet impinges on it. This measured radial pressure distribution is then compared with pressure profiles predicted by the present calculations. Model predictions are compared with experimental results at three different current levels.

5.4.3 Formulation

A methodology similar to that adopted in the investigation of plasma flows in arcjet thrusters described earlier, is used in the study of the plasma jet in the present work. A 2-D axisymmetric model is used and the calculations are carried out in two

stages. The internal and external flows are described by the same set of governing equations as described in Chapter II, except that, the boundary conditions for the two are different. An internal flow simulation is first conducted in order to obtain the flow field, temperature and species concentration within the torch body for a given mass-flow rate and power. The calculated exit plane values of the flow variables are then used as boundary conditions for the external flow calculations of the plasma jet. The predicted radial pressure profile is then compared with experimentally measured pressure profiles at the surface of a water-cooled copper workpiece [60]. The internal flow simulations provide profiles of the flow variables at the exit plane of the torch. This enables investigation of the effects of torch geometry on the temperature and velocity fields at the exit plane of the torch, and allows us to explore their effects on the external jet.

Assumptions

The above paragraph has outlined the broad framework adopted in the present study of plasma flows in these torches. Arc welding is a highly complex phenomenon. It involves a close coupling of several effects including electromagnetic forces, fluid flow - both molten and gaseous phases. From the practical standpoint, the development of thermal stresses and stress-induced deformation are of importance as they affect the properties of the weldment. To make the problem tractable however, some simplifying assumptions are made in addition to the general assumptions discussed earlier. In the present work, emphasis is placed only on the plasma jet impinging on the workpiece. Phase-change at the welding surface is not taken into consideration. This work does not couple modeling of the weld pool with the arc. The workpiece is considered a boundary of the fluid domain. Self-induced magnetic fields are included and buoyancy

Figure 5.24: Geometry of the Plasma Torch for internal flow simulations.

effects are neglected. Argon (Ar) is the plasma gas as well as the shield gas. It is assumed that the gas comprises of Ar , Ar^+ , and e^- and hence the only “reaction” considered is:

The plasma is assumed to be quasi-neutral i.e. the effect of charge separation is neglected since the Debye lengths are much smaller than the characteristic dimensions involved. Figure 5.24 shows the physical domain under consideration for the internal flow.

Internal Flow - Boundary Conditions

The non-dimensional form of the governing equations described in Chapter II are solved in conjunction with appropriate boundary and initial conditions to obtain the distributions of velocity, temperature, magnetic induction and species concentrations within the torch.

Figure 5.25: Computational Domain for Electromagnetics (Model I)

All the boundary conditions for the flow variables are identical to those discussed in the case of the hydrogen arcjet except at the anode wall. To simulate the external cooling of the torch body, a convective boundary condition of the form (non-dimensionalized) $dT/dr|_{wall} = -h_{eff}(T|_{wall} - T_{cool})$ is used. h_{eff} is set to 175 (dimensional value, $h_{eff} = 3.47\text{e-}2 \text{ m}^{-1}$ and T_{cool} is set equal to 300 K. The water temperature cooling the torch in the experiments was at room temperature and hence T_{cool} is fixed at 300 K. The value of h_{eff} was chosen to limit wall temperatures close to 3000 K. The mass density and the electron number density at the wall are determined by setting the first derivative of each of these quantities to zero. This prescription was found to be most stable numerically.

The boundary conditions for the electromagnetics differ from those discussed earlier for the arcjet. As shown in Figure 5.24 the nozzle does not have a diverging region. Two different models for the electromagnetic computations were studied. The computational domain for each of these is shown in Figure 5.25 and 5.26. In

Figure 5.26: Computational Domain for Electromagnetics (Model II)

the first model, the electromagnetic calculations commence from the axial location corresponding to the beginning of the straight section. Thus, the electromagnetic calculations commence at an axial station that is ≈ 2.85 mm upstream from the exit plane of the torch. At this axial location, (the vertical plane CX in figure 5.25) the radial current density, j_r is set to zero, which is tantamount to setting $\partial B/\partial x = 0$. A constant value of B_θ depending on the operating current, is prescribed along the straight section of the nozzle. In other words $B_\theta = \mu_o I / 2\pi r_c$, where r_c is the inside radius of the torch nozzle body. $B_\theta = 0$ along the centerline, by symmetry and $\partial B/\partial x = 0$ along the exit plane. These boundary conditions mimic a transferred arc quite well. The presence of the pilot arc is not included. The Neumann boundary conditions applied along plane CX and at the exit plane, make the current lines parallel to the centerline and the prescription of a fixed value of B_θ along the inside radius of the constricting nozzle prevents any current attachment on the walls.

	ABCD (Anode)	DE (Exit Plane)	EF (Centerline)	FGH (Cathode)	HA (Inlet)
ρ	$\partial\rho/\partial r = 0$	from P_{exit}	$\partial\rho/\partial r = 0$	$\partial^2\rho/\partial r^2 = 0$	Equation of state
u	$= 0$	$\partial^2 u/\partial x^2 = 0$	$= 0$	$= 0$	$u = 0$
w	$= 0$	$\partial^2 w/\partial x^2 = 0$	$\partial w/\partial r = 0$	$= 0$	$\partial^2 w/\partial x^2 = 0$
T	$\partial T/\partial r =$ $-h(T_{r=r_o} - T_{wall})$	$\partial^2 T/\partial x^2 = 0$	$\partial T/\partial r = 0$	$\partial^2 T/\partial r^2 = 0$	from T_o
n_e	$\partial^2 n_e/\partial r^2 = 0$	$\partial^2 n_e/\partial x^2 = 0$	$\partial n_e/\partial r = 0$	$\partial^2 n_e/\partial r^2 = 0$	$\partial^2 n_e/\partial x^2 = 0$

Table 5.4: Boundary conditions for internal flow variables in a plasma torch

In the second model, the electromagnetic computations begin from the axial location corresponding to the beginning of the sloping face of the cathode (segment GF in figure 5.26). This corresponds to a distance of 4.58 mm upstream from the exit plane of the torch. Along the cathode surface, i.e. GF, the total enclosed current is assumed to decrease linearly from the prescribed current at G to zero at F. As a result of such a boundary condition, B_θ along GF remains at a constant value. Along segment GA and AB, the enclosed current is assumed to be fixed. Hence, along GA and AB, B_{theta} scales inversely with the radius. Along the centerline, B_{theta} is set equal to zero and along the exit plane $\partial B/\partial x = 0$ as in the previous model. These two electromagnetic models were studied to assess the impact of the arc models on the exit plane values, and their final impact on the external flow solutions for a given mass flow rate, power-level and current. The boundary conditions described above are summarized in Tables 5.4 and 5.5.

External Flow - Boundary conditions

The exit plane values of all the flow variables calculated from the internal flow

	CD	DE	EX	CX
B_θ	Prescribed	$j_r = 0$	$B_\theta = 0$	$j_r = 0$

Table 5.5: Boundary conditions for electromagnetics (Model I)

	AB	AG	GF	FX
B_θ	Prescribed	Prescribed	Prescribed	$B_\theta = 0$

Table 5.6: Boundary conditions for electromagnetics (Model II)

solutions are used as inflow boundary conditions for the external flow, up to the radial location corresponding to the dimensions of the nozzle (along AB in Figure 5.27). BC in Figure 5.27 denotes the portion of the domain simulating the flowing shield gas. Shield gas flow is simulated by prescribing a profile for the axial and radial components of velocities so as to match the total shield gas mass flow rate in the experiments. Along BC in Figure 5.27, the pressure is set equal to one atmosphere. Based on this value of pressure, and a prescribed shield gas temperature, the density is fixed. The integrated mass flow rate of the shield gas is thus set to correspond to the experimentally reported shield gas volume flow rate (≈ 25 standard cubic feet/hour (SCFH)). A reasonable value for the temperature and density need to be prescribed for the shield gases. Our calculations indicated however, that these profiles have a negligible influence on the solution. Variations in shield gas flow rate also have minimal effect on the overall solution. It was seen that doubling the shield gas flow rate led to a change of less than 2% in the peak predicted pressure at the surface of the work-piece. The edge of the torch body (denoted by CD in Figure 5.27) is

Figure 5.27: Physical Domain for simulation of Plasma Jet issuing from the torch.

maintained at a fixed temperature and atmospheric pressure. In these simulations the torch body is maintained at 500 K, but the overall solution is fairly insensitive to this value of temperature. Symmetry boundary conditions, i.e., $\partial\phi/\partial r|_{r=0} = 0$ are prescribed along the centerline (AF in Figure 5.27) for all variables except the azimuthal and the radial components of velocity. The radial and swirl components of velocity are set to zero along the centerline, consistent with symmetry considerations along the centerline.

At the plate surface (FE in Figure 5.27), no-slip conditions are applied for all components of velocity. A convective boundary condition is used for the temperature, which in non-dimensional form is as follows: $\partial T/\partial x|_{x=L} = -h_{eff} (T_{x=L} - T_c)$, where $h_{eff} = h_o \exp(-r/r_o)^2$, $T_c = 500$ K. $h_o = 75$ (dimensional value of 0.01488 m^{-1}) and $(r/r_o)^2$ is the normalized distance from the centerline along the plate surface. The algebraic form of the heat-transfer coefficient was found to influence the radial pressure profile. The present form exhibits the best results in capturing the steep

radial temperature gradient along the surface of the workpiece, expected in experiments. The first derivatives of mass density and electron number density are set to zero at the workpiece. The radial location corresponding to the edge of the torch body is the outer boundary of the computational domain in the radial direction (DE in Figure 5.27).

Implicit extrapolation in the radial direction is used along DE to describe all velocity components and species (i.e. $\partial^2 \phi / \partial r^2|_{r=r_o} = 0$). Static pressure along this plane is set equal to the ambient atmospheric pressure. An insulated boundary condition is used to describe the temperature at the outer radial boundary, i.e. $\partial T / \partial r = 0$. Since the size of the computational domain chosen is large enough, such a boundary condition does not affect the solution. Specification of a constant temperature along the outer radial boundary is found (a posteriori) to influence the solution and is therefore not used. Electron number density at this radial outflow boundary is obtained by setting its second derivative to zero in the radial direction. The equation of state is used to determine the mass density. In non-dimensional form, this can be written as $\rho = P_{atm} / T_{r=r_o} - n_e$.

The governing equation describing the B_θ field is the same as in the internal flow. However, in the interest of obtaining high computational speeds, the magnetic transport equation is not solved over the entire domain. It has been observed experimentally that the spread of the jet in the radial direction is negligible. Hence the extent of the computational domain for the electromagnetics is restricted to twice the extent of the nozzle radius (AceF denotes the region over which the magnetic transport equation is solved). A restricted domain describing the electromagnetics has the virtue of reducing computing time. It is assumed that no current flows along

	AD	DE (Outflow)	EF (Workpiece)	FA (Centerline)
ρ	Prescribed	$\partial^2 \rho / \partial r^2 = 0$	$\partial \rho / \partial x = 0$	$\partial \rho / \partial r = 0$
u	Prescribed	$\partial^2 u / \partial r^2 = 0$	$= 0$	$= 0$
w	Prescribed	$\partial^2 w / \partial r^2 = 0$	$= 0$	$\partial w / \partial r = 0$
T	Prescribed	$\partial T / \partial r = 0$	$\partial T / \partial x =$ $h(T_{r=r_o} - T_{plate})$	$\partial T / \partial r = 0$
n_e	Prescribed	$\partial^2 n_e / \partial r^2 = 0$	$\partial n_e / \partial x = 0$	$\partial n_e / \partial r = 0$

Table 5.7: Boundary conditions for external flow variables

	AB	Bc	ce	eF	FA
B_θ	Prescribed	$B_\theta = \mu_o / 2\pi r$	$B_\theta = \mu_o / 2\pi r_{r=r_c}$	$j_r = 0$	$B_\theta = 0$

Table 5.8: Boundary conditions for electromagnetics

the surface of the work-piece, which translates to $\partial B / \partial x = 0$, (i.e., $j_r = 0$). $B_\theta = 0$ is used along the centerline (which is identically true by symmetry). Values of B_θ obtained from the internal flow solutions are prescribed along the surface AB (see Figure 5.27), up to grid locations less than the nozzle radius. Along the remaining radial grid points the enclosed current is assumed to be constant (i.e. $B_\theta = \mu_o I / 2\pi r$ along Bc in Figure 5.27). The constant value of enclosed current corresponding to the location 'c' is prescribed along 'ce' in Figure 5.27. Thus a constant value of B_θ was maintained along 'ce'.

The boundary conditions described above are summarized in Tables 5.7 and 5.8.

Initial Conditions

As in the case of the arcjet simulations, reasonable initial profiles need to be specified for the internal and external flow simulations. The initial profiles describing flow variables in the internal flow simulations are similar to those used for the arcjet. The initial conditions for the external flow are found to be not very crucial for stable time-marching. Small values are prescribed for the axial and radial components of velocities throughout the domain ($u \approx 20\text{m/s}$, $w \approx 20\text{ m/s}$). The static pressure within the domain is set at the ambient value. The initial temperature is kept at 10000 K throughout the domain. The electron number density was set at a small constant value all through the domain (dimensional values of $7.8\text{e}18\text{ m}^{-3}$). The density is evaluated from the temperature and pressure using the equation of state. In non-dimensional form this is written as $\rho = P_{atm}/T - n_e$.

5.4.4 Artificial Dissipation

The form of the term describing artificial dissipation is similar to that used in modeling arcjet thrusters (i.e. $\mu_r \partial^2 \phi / \partial r^2 + \mu_x \partial^2 \phi / \partial x^2$), however the algebraic expressions for μ_x and μ_r were different. These coefficients are defined differently for governing equations describing internal and external flows. For internal flow, these are:

$$\mu_{r_{exp}} = \begin{cases} 0.00025\rho dr & \text{for } T \leq 2000K \\ 0.005\rho dr & \text{for } 2000K \leq T \leq 1000K \\ 0.025\rho dr & \text{for } T \geq 10000K \end{cases}$$

and

$$\mu_{r_{imp}} = 5e - 6/dr$$

$$\mu_{x_{exp}} = \begin{cases} 0.05\sqrt{T}dx & \text{for } T \leq 10000K \\ 0.025\sqrt{T}dx & \text{for } T \geq 10000K \end{cases}$$

$$\mu_{x_{imp}} = \begin{cases} 0.0025\sqrt{T}dx & \text{for } T \leq 2000K \\ 0.00025\sqrt{T}dx & \text{for } T \geq 2000K \end{cases}$$

Co-efficients in the artificial dissipation term in the external flow were as follows:

$$\mu_{r_{exp}} = \begin{cases} 0.0005\rho dr & \text{for } T \leq 2000K \\ 0.005\rho dr & \text{for } 2000K \leq T \leq 1000K \\ 0.025\rho dr & \text{for } T \geq 10000K \end{cases}$$

and

$$\mu_{r_{imp}} = 2.5e - 3/dr$$

$$\mu_{x_{exp}} = \begin{cases} \sqrt{T}dx & \text{for } T \leq 2000K \\ 0.05\sqrt{T}dx & \text{for } 2000K \leq T \leq 1000K \\ 0.05\sqrt{T}dx & \text{for } T \geq 10000K \end{cases}$$

$$\mu_{x_{imp}} = \begin{cases} 0.1\sqrt{T}dx & \text{for } T \leq 2000K \\ 0.0005\sqrt{T}dx & \text{for } 2000K \leq T \leq 1000K \\ 0.00025\sqrt{T}dx & \text{for } T \geq 10000K \end{cases}$$

The important difference between the coefficients, μ_r and μ_x used in arcjet simulations and those used in plasma flows in torches is that the implicit term is less than the explicit term in the plasma torches. Additionally, the algebraic forms of the coefficients are dependent on temperature. This model is found to be most stable numerically. Flow regimes are categorized into three regions. $T \leq 2000K$ represent cold regions of the flow - regions close to the inlet plane in the internal flow and regions close to the torch body in the external flow. Regions close to the core of the arc are characterized by temperatures between 2000 K and 10000 K, both in the internal and external flows. Temperatures above 10000 K are typical of the arc core. In the colder regions, where the mass-density is high, μ_r has a smaller constant multiplicative value as compared to the hotter regions which have a lower mass-density. Constant multiplicative factors for the implicit and explicit terms in the axial directions also

scale with temperature. The constant multiplicative factors are obtained by trial and error. They are based on the idea that insufficient dissipation leads to unphysical values of the dependent variables and instability during time-marching. Location of the maximum and minimum values of temperature, pressure and velocity in the computational domain are monitored during the time-marching. The multiplicative factors are varied only in those regions where the minimum values are unphysical. This method, though ad-hoc, provides very good guidance on how to vary numerical dissipation. The above dissipation model is used to study the 100 A case. The coefficients in the implicit and explicit terms have to be increased by a factor of 2 or 3 to study the 125 A and 150 A case. This shows that the artificial dissipation model is general and only minor changes in the coefficients yield stable solutions for three different current levels.

5.4.5 Results

The physical domain for the internal flow calculations consist of a portion extending about 8 mm inwards from the exit plane of the torch. The cathode tip is approximately 3 mm from the exit plane (see Figure 5.24). This portion of the torch has chosen since it is important to model the region before the plasma gas encounters the arc. The cold gas flow through the entire torch assembly is not modeled. The results of the present simulation are compared with experiments conducted in the Industrial, Systems and Welding Engineering Department (ISWE) at OSU [60].

In the experiments, a radial profile of the static pressure (gage) at the surface of a water-cooled copper plate was measured for different operating current levels by scanning the plasma torch over a water-cooled plate, with a pressure tap. The results

of present simulations are compared with these experimental pressure traces obtained for three different current levels (100 A, 125 A and 150 A).

Such a comparison requires precise knowledge of the stagnation pressure (and hence mass flow rate), power level and current. Except for the current, exact experimental values for power level and mass flow rate could not be obtained in the experiments. The volume flow rate of the plasma and shield gases were measured far upstream of the torch exit. The numerical formulation used in this work requires the specification of a stagnation pressure to obtain a specific mass flow rate. To match the experimental conditions as closely as possible, the simulations aimed at obtaining a mass-flow rate corresponding to the experimental value based on the volume flow rate at a temperature of 300 K. The power level is obtained a posterior, as discussed in the case of arcjets.

Internal and external flow simulations were performed for each of the current levels. The magnitudes of the stagnation pressure and the specific model describing the arc do impact the values of the flow variables at the exit plane. These in turn, impact the predicted pressure profile at the workpiece, since the exit plane values (obtained from the internal flow simulations) are used as boundary conditions for the external flow simulations. These effects are investigated by conducting three sets of simulations which are summarized in Table 5.9.

Comparison of the predicted pressure profiles based on case I and case II show effects of the arc model on the solution (for a given stagnation pressure, and power

t

	Current (A)	P_o	Arc Model	Power (KW)
Case I	Fixed	P_1	Model I	Fixed
Case II	Fixed	P_1	Model II	Fixed
Case III	Fixed	P_2	Model II	Fixed

Table 5.9: Case studies for the Plasma Torch

	Current (A)	P_o in. of water	Arc Model	Power (KW)
Case I	100	40	Model I	≈ 2.1
Case II	100	40	Model II	≈ 2.1
Case III	100	30	Model II	≈ 2.1

Table 5.10: Operating conditions for the different case studies

and current level), while comparison of case II and case III show the effects of stagnation pressure (for a given arc model, power and current level). The above sets of simulations were performed for current levels of 100 A, 125 A and 150 A.

In this section, results for the 100 A case are presented. The power level, stagnation pressures and current level for this case are given below.

The results of simulations for the above cases are compared with experimental conditions listed in Table 5.11.

The predicted power level in the simulations (100 A case) is about 2.1 KW (close to the experimental conditions). This is obtained by setting the conductivity floor at 1000 mho/m. The simulations are run on a Silicon Graphics Challenger L workstation.

Polarity	Straight
Plasma Gas	Argon
Shield Gas	Argon
Plasma Gas flow rate (CFH)	≈ 13
Shield Gas flow rate (CFH)	35
Current (Amps)	100
Stand-off Distance (in.)	3/8
Power (KW)	≈ 2.2

Table 5.11: Experimental Conditions

A uniform 50×32 grid is used in this simulation of the internal flow, and converged solutions are obtained in about 12-15 hours of CPU time.

The computational domain for the external flow extends from the centerline up to the edge of the torch body and from the exit plane of the torch to the work-piece. Physically, it is a rectangle of dimensions 9.5 mm by 12.7 mm. The boundary of the computational domain (along the torch exit plane) is split into three regions - surface AB comprising the exit plane of the torch, surface BC representing the shield gases and surface CD being the region along the solid torch body (see Fig 5.27). A uniform 30×80 grid is used in this computation. The simulations are also run on a Silicon Graphics Challenger L workstation, and converged solutions are obtained in about 15 hours of CPU time. Since the results of the simulation are compared against gage pressures-between 30 to 60 inches of water, it was necessary to ensure convergence of the non-dimensional quantities to at least 4 decimal places.

Figure 5.28: Current Contours within the plasma torch (Model I)

Results for Internal and External Flow

Results for the 100 A case with two different arc models and two different stagnation pressures are presented in this section. Figure 5.28 shows the current contours within the torch for model I whereas, Figure 5.29 shows the current contours for the second model. It can be seen that both these models mimic the arc discharge very well. In model II the arc emanates from the cathode and models the energy addition to the gas stream more realistically, whereas in model I the arc is modeled only in the straight section of the torch. The impact of the arc model on the exit plane and centerline profiles is discussed next. In all the figures comparing the effects of the arc model, curves with asterisks joined by a line represent results for model I and curves with circles joined by a line represent results for model II. Figures 5.30 and 5.31 show the velocity and temperature profiles along the centerline, respectively. It can be seen that the cold plasma gas is moving at a low velocity, till it encounters the hot

Figure 5.29: Current Contours within the plasma torch (Model II)

arc region. The energy gained from the arc (by Ohmic heating) accelerates the gas and also raises its temperature considerably.

This energy addition to the gas brings about ionization of the cold gas as can be seen in Fig 5.32 depicting the variation of the ionization-fraction (α) along the centerline. It is interesting to note that the plasma gas is fully ionized along the centerline in the region of the arc. This implies that doubly ionized argon atoms Ar^{++} should be present, although these have not been included in the calculations. It can be seen that the velocities predicted by model II are higher than those predicted by model I. Model II predicts a temperature rise at an earlier axial location, as the gas “encounters” the arc earlier. However, since the power level in both the cases are the same, the maximum temperature predicted by both the models are nearly equal. Qualitatively, both models predict similar profiles. The temperature rise is steep initially and then tapers off towards the exit plane. It is seen that both models predict complete ionization along the centerline in the region where the arc is modeled.

Figure 5.30: Centerline Axial Velocity Profiles

Figures 5.33 and 5.34 depict the radial variation of axial velocity and temperature along the exit plane. Steep gradients in velocity and temperature are seen in regions close to the centerline. The gradients are less steep in regions further away from the centerline, in both models. As expected, the temperature profiles predicted by both models are nearly the same. The velocity profiles are qualitatively the same, although, the velocities predicted by model II are higher than those predicted by model I. These observations are consistent with the centerline profiles discussed earlier. Figure 5.35 shows the plasma temperature profile along the inner surface of the anode. It can be seen that the temperature remains fairly constant till the flow encounters the region close to the arc where it rises rapidly to about 3000 K. These gas temperatures are not

Figure 5.31: Centerline Temperature Profiles

unrealistic as the inner surface of the nozzle undergoes a considerable amount of deterioration. The wall temperature profiles predicted by both models are qualitatively the same.

The effect of stagnation pressure on the centerline and exit plane profiles of temperature and velocity are discussed next. In all the figures, curves with circles joined by a line represent results for a stagnation pressure of 30 inches of water (gage) whereas, the curves with asterisks joined by a line represent results for a stagnation pressure of 40 inches of water. Lowering the stagnation pressure, lowers the mass flow rate of the plasma gas. Since the power levels are the same, a smaller mass-flow rate yields higher temperatures. However, this difference is not marked. This is depicted

Figure 5.32: Centerline Ionization Fraction Profile

in Figure 5.37. A similar trend is seen along the exit plane (see Fig 5.38). Higher velocity is predicted for the case with a higher stagnation pressure. This is observed along the centerline and the exit plane (Figs. 5.36 and 5.39).

In all the simulations (with different arc models and different stagnation pressures), the qualitative aspects of the temperature and velocity profiles along the exit plane and the centerline are the same.

Figures 5.40 and 5.41 show contours of temperature and ionization fraction, respectively in the plasma torch. The region close to the centerline consists of the hot core. A high degree ionization is expected in this region as shown in Figure 5.41.

Figure 5.33: Radial profiles of axial velocity at the exit plane of the plasma torch

Figure 5.34: Radial profiles of Temperature at the exit plane of the plasma torch

Figure 5.35: Temperature of the plasma along the inner surface of the torch body

Figure 5.36: Centerline Axial Velocity Profiles

Figure 5.37: Centerline Temperature Profiles

Figure 5.38: Radial profiles of Temperature at the exit plane of the plasma torch

Figure 5.39: Radial profiles of Axial Velocity at the exit plane of the plasma torch

Figure 5.40: Temperature contours in the plasma torch. Innermost contour is $T=20,000$ K, the outermost is $T = 12,000$ K. Each contour is incremented by $1,600$ K

Figure 5.41: Ionization fraction in the plasma torch. Innermost contour is $\alpha = 1.0$, the outermost is $\alpha = 0.2$. Each contour is incremented by 0.2

Similar trends for centerline and exit plane quantities were observed for the 125 A and 150 A simulations.

Figure 5.42 shows velocity vectors in the external flow. Temperature contours are shown in Figure 5.43. It can be seen that plasma jet spreads very little. This is due to the high velocity of the jet exiting the torch and the small stand-off distance. The innermost contour shows the high temperature regions (temperatures above 8000) in the arc. The turning of the hot gas flow is illustrated by these two plots.

Figure 5.44 displays the growth of the wall jet. It can be seen that with radially increasing distances from the centerline, the maximum radial velocity increases up to a point and then decreases thereafter. Also the location of the maximum velocity in each of the radial velocity profiles occurs further away from the workpiece (stagnation plane) with increasing radial distance from the centerline. These are typical characteristics of wall jets [61].

Figure 5.42: Velocity Vectors in the external flow of the plasma jet. For clarity, velocity vectors along alternate grid points have been plotted in the axial direction and every fourth grid point has been plotted in the radial direction

Figure 5.45 shows the temperature of the gas along radial outflow boundary (along DE in Figure 5.27). It is seen that the temperatures near the workpiece are high but drop off sharply with increasing distance from the workpiece. Figure 5.46 shows a comparison of the static pressure profile obtained experimentally (the only quantity measured in the OSU experiments) and that obtained from the present simulations. The pressure profile obtained experimentally shows that the plasma jet tends to remain collimated. It is seen that the arc pressure (gage) drops sharply to values close to zero within a distance of about three times the nozzle radius from the centerline. It is seen that model II with a stagnation pressure corresponding to 40 inches of water (gage) predicts a higher pressure as compared to model II with a stagnation pressure of 30 inches of water. The peak predicted pressure for the different stagnation pressures and models differ by about 3 inches. This is close to the experimental error

Figure 5.43: Temperature Contours in the external jet. The innermost is $T = 8000$ K, and the outermost is $T = 2000$ K. Each contour is incremented by 1,200 K.

which is about 1-2 inches of water (Figure 5.46). The simulations predict a broader pressure profile as compared to the experiment. It is seen that the different models and stagnation pressures do not drastically impact width of the pressure distribution. Overall, the agreement with experiment is very good.

Comparison of pressure profiles along the workpiece for a current level of 150 A is shown in fig 5.47. It is seen from the 100 A and the 150 A case, that a difference of 10 inches of water (gage) in the stagnation pressure gives about a 10% difference in the peak values of the predicted pressure at the workpiece. The qualitative trends for the different arc models and stagnation pressures are the same for both the current levels.

The pressure profiles predicted by the simulations match the experiments very well. It is seen that model I also predicts the pressure profile well. Such a model

Figure 5.44: Radial component of velocity in the plasma torch external flow at five radial locations: $r=0\text{mm}$, $r=3.175\text{mm}$, $r=6.35\text{mm}$, $r=9.525\text{mm}$ and $r=12.7\text{mm}$.

is useful in generating the initial guess as a reduced computational domain for electromagnetic computations reduces computing time. The steep drop off in the profile is not captured very well by the simulations in regions very close to the centerline. This could be a combination of the following factors; simple heat transfer model at the surface of the work-piece, predicted exit-plane values of the plasma jet and the effects of artificial dissipation.

Figure 5.45: Temperature profile at the edge of the computational domain in the external flow, $r=12.7\text{mm}$

Discussion of results

The current contours in the internal flow (see Figures 5.28 and 5.29) depict the current flow that is expected in such plasma arcs where the stand-off distance is small. The high velocities at the exit plane and the small stand-off distance restrains the arc from expanding. This is important for concentration of the heat load on the workpiece so as to obtain maximum penetration of the weld pool and obtain the keyholing effect. The heating of a subsonic flow leads to its acceleration. The axial velocity profile along the centerline shows this effect rather well. Based on these velocities, the residence time of the gas in the region of the arc is on the order of a few microseconds. These

Figure 5.46: Comparison of the radial distribution of static pressure along the surface of the workpiece with experimental data from [60]. The stagnation pressures (gage) in inches of water are given in the parenthesis.

relatively long residence times allow the gas to proceed towards thermal equilibrium and full ionization. The sharp drop off in the radial temperature distribution at the exit plane (Fig. 5.34) in regions close to the centerline is due to the high degree of ionization.

The temperature contours representing the temperature field in the external jet closely follow the velocity vectors representing the flow. These contours also show that the hot core of the jet does not expand very much. The predicted pressure profiles although exhibiting good agreement with experiments do not completely capture the steep drop off shown by experiments. The experimental data show that $dp/dr|_{x=L}$ is

Figure 5.47: Comparison of the radial distribution of static pressure along the surface of the workpiece with experimental data from [60]. (150 A)

negative and large in regions close to the centerline. This behaviour could be possibly due to the shape of velocity profile issuing out of the plasma torch and the cooling of the plate. It is possible that the drop-off in the real axial velocity profile along the exit plane may be steeper than that predicted by the internal flow simulation. This could impact the shapes of the radial pressure profiles predicted by simulation and those observed experimentally. Another possible reason is the cooling of the plate. The cooling of the plate was simulated by a convective boundary condition with a radially varying heat-transfer coefficient. Since $P = n_T kT$, the following analysis is

likely to explain the difference in shapes of the pressure profiles close to the centerline.

$$\frac{dP}{dr} = n_T k \frac{dT}{dr} + kT \frac{dn_T}{dr}$$

As can be seen from the above equation, dP/dr is zero at the centerline, however, the shape of the profile depends on the radial slopes of temperature and total number density and temperature and total number density. All these quantities at the plate surface depend on the cooling of the plate. Our model is unable to capture this effect in regions close to the centerline along the plate surface. Varying h_o and α did not affect the shape of the pressure profile in that region. A more elaborate heat-transfer model is probably needed to model the cooling of the plate in regions close to the centerline. Lastly, the effects of artificial dissipation could also lead to the flatness of the pressure profile in regions close to the centerline. A case study for the 100 A case, in which the artificial dissipation in regions with temperature greater than 10,000 K was increased tenfold, showed that the peak pressure dropped and the width of the pressure profile increased.

5.5 Summary and Conclusions

The LBI scheme has been extended to model reacting flows in the present work. Modeling of reacting flows entails a solution of the compressible Navier-Stokes equations, master equations and Maxwell's equations. The versatility of the numerical scheme and the model used in the present work is demonstrated by its ability to predict characteristics of different discharges. The implicit scheme used in the present work has demonstrated good potential in handling stiffness problems which characterize reacting flows. Further, the present work has shown that numerical simulations of plasma and reacting flows can be carried out on modern computers in reasonable

amounts of CPU time. The model has been successfully applied to study flows in arcjet thrusters and plasma torches and the results of these simulations have been compared with experimental data. Converged solutions for arcjet flows have been obtained in about 10-15 hours of CPU time in the uniprocessor mode on the CRAY Y-MP. Converged solutions for the internal and external flow in plasma torches have been obtained in about 10-15 hours on Silicon graphics workstations.

Characteristics of flow in a 1 KW arcjet thruster have been studied with two different arc attachments. Results of these simulations have been compared with experimental data from two different groups for supposedly identical operating conditions. The overall agreement with experimental data is good. The question of uniqueness of arc attachment in the two experiments has been raised and the importance of correctly predicting the energy loading of the propellant stream as well as its effects on the exit plane profiles have been highlighted. The two main weaknesses in the present physical model are its inability to predict a constricted arc and the assumption of a single temperature. The assumption of a single temperature has been shown to be capable of providing reasonably accurate solutions. However, a more realistic description of the plasma requires the inclusion of an equation describing the EEDF. The need to add artificial dissipation to enable stable time-marching is a weakness associated with the numerical scheme. Limited parametric studies have shown that overall impact of numerical dissipation on the accuracy of the solution is however less than 10%.

This work is the first attempt to model transferred plasma arcs. Internal flow in a welding torch and the external flow of the plasma jet impinging on the workpiece have been modeled. The agreement between experimental data and the results of

these simulations is very good. Artificial dissipation is an important parameter in low speed flows and can impact the numerical solution. This highlights the need to develop sound and universal models for artificial dissipation which have a minimal effect on the accuracy of the solution.

The LBI method has been shown to be extremely versatile in handling low speed (as in the plasma welding torches) and high speed (as in the arcjet) plasma flows. It is however capable of much more. Given the level of success as demonstrated by the results in this chapter, a framework for modeling flowing molecular plasmas is devised in the next chapter. A necessary first step in constructing this framework is the inclusion of molecular vibrational energy exchange processes on a state-specific (i.e. as a function of vibrational state or quantum number) basis. This is described next, along with the influence of vibrational non-equilibrium on the energy distribution of electrons.

CHAPTER 6

METHODOLOGY FOR MODELING MOLECULAR DISCHARGES

6.1 Introduction

This work is aimed at developing tools to realistically model reacting and plasma flows. With this goal in mind, an implicit algorithm capable of handling stiff systems of equations has been selected for numerical solutions of equations describing such reacting and plasma flows. The LBI scheme, originally developed to solve unsteady, compressible Navier-Stokes equations has been extended in this work to study complex plasma flows. A single temperature description of the flowing plasma has been used. Chemical kinetics and electromagnetic effects have been coupled with equations describing the flow, self-consistently. Internal and external plasma flows in welding torches and internal flows in arcjet thrusters were studied using this method. To the best of this author's knowledge this is the first complete simulation of internal and external flows describing a transferred plasma arc in 2-D. The results of these simulations have been compared with experimental measurements and show good agreement. The numerical scheme and the plasma model have also been used to study the characteristics of internal flows in a 1 KW hydrogen arcjet thruster. The predicted results from this simulation also compare well with experiments.

The experience gained by studying these different discharges has laid the foundation to attempt a realistic description of flowing molecular plasmas. This involves coupling the energy equation (described in Chapter II) with a Boltzmann equation describing the EEDF for the distribution of electron energies. Such an approach is necessary when modeling electrical discharges containing tightly bound molecular species such as N_2 , CO , etc. The electron energies in such environments are described by a Boltzmann-like equation coupled to the vibrational states of these molecules. However, numerical simulation of a system of equations describing such non-equilibrium plasmas is a daunting task and places stringent demands on the speed and memory resources of the computing system. Moreover, computing time is a major factor that requires consideration in such an effort. The high-performance feature and the implicit nature of the numerical scheme used in this work, raises the possibility of greatly reducing the computational time required in such a study. Research on plasma flows at The Ohio State University (of which the present work is a part) has proceeded to approach this goal in a systematic manner, by studying models with increasing levels of detail. The methodology to model flowing molecular plasmas incorporating the aforementioned effects is described in the next section.

6.2 Methodology

6.2.1 Introduction

In contrast to atomic plasmas, molecular plasmas introduce additional inelastic processes. Specifically the energies of electrons in a molecular discharge couple very well with the vibrational states of tightly bound diatomic species via inelastic collisions. Consequently, in systems where V-V exchange collisions dominate V-T

exchanges, the vibrational modes of molecular motion are out of equilibrium with the translational mode. This in turn causes the electron energies to also be out of equilibrium with the translational modes of the gas particles, and to be non-Boltzmann without a clearly definable average electron energy. The rate at which these inelastic collisional processes occur is governed by their respective time constants.

At this juncture, it is appropriate to discuss the relevant time-scales and “ideal” flow situations corresponding to these time-scales. There are in general, two main time-scales in connection with flows, namely, the convective time-scale and the viscous diffusive time-scales. The convective time-scale is defined as the ratio of a characteristic length of a given geometical configuration to the local flow velocity. Similarly, the diffusive time-scale is defined as the ratio of the square of the characteristic length to the kinematic viscosity. Where there are severe gradients in the flow variables or where time scales for processes are comparable to the local convective time scale, the concept of classical thermodynamic equilibrium is not applicable. However, a fairly loose criterion, called “Local Thermodynamic Equilibrium” or (LTE) is used commonly to model such flows. This is the basis of classical Fluid Dynamics and Heat Transfer. LTE is used to describe situations wherein the time scales for all processes are infinitely smaller than the smaller of the convective or diffusive time-scales. Another limiting case is that of “frozen flow”, wherein, microscopic processes proceed at time-scales infinitely longer than the convective or diffusive time-scales. Between these two extreme ideal cases, lie real engineering processes which proceed at a pace comparable to the convective or diffusive time scales. These processes are termed as “non-equilibrium” processes.

It is possible for different regions of a flow to comprise of processes which are “frozen”, in LTE or out of equilibrium. Flowing plasmas or electrical discharges are usually in a state of non-equilibrium. The distinguishing feature of non-equilibrium plasmas is the difference in the mean energies of the electrons and heavy species arising from elastic and inelastic collisions. This is especially true in the case of low-pressure discharges. Various reactive processes (dissociation, ionization, recombination, etc.) taking place in flowing plasmas are also out of equilibrium and hence must be described in terms of finite reaction rates. In addition to chemical non-equilibrium, the internal modes of the various species can be out of equilibrium with the external modes. Such internal mode disequilibrium is described by rate equations (master equations) governing the various state-to-state transitions. This involves treating each of the internal states of a specie as a separate entity, governed by its own master equation. A rigorous description of flowing plasmas requires coupling of the EEDF with various internal states. This is necessary since the EEDF controls the chemistry through the various reaction rates which depend on electron energies and populations of specific excited states. Thus, the EEDF determines the characteristics of the plasma. A deeper understanding of flowing plasmas in discharges can be obtained by a fully coupled approach which involves the flow, electromagnetics, heavy particle energy equation, master equations governing chemical kinetics and a governing equation for the EEDF.

Evaluation of the EEDF in discharges is a topic of current interest in the study of molecular plasmas [11]. Knowledge of the EEDF is an important step in developing techniques that can quantitatively simulate discharges used in a number of commercial

applications. The following section describes a typical problem in which the plasma is in a state of vibrational non-equilibrium.

6.2.2 Arcjet Flows with Vibrational Non-equilibrium

Flows in arcjet thrusters with propellant such as Nitrogen (N_2), Ammonia (NH_3) or Hydrazine (N_2H_4) are most likely to be in a state of vibrational non-equilibrium. This occurs because the vibrational states of molecules such as Nitrogen are easily excited by electron impact and by anharmonic V-V pumping, where the vibrational quanta are exchanged via collisions. Discharges involving gases such as Nitrogen, high V-V pumping rates and rapid electron impact excitation of vibrational modes are accompanied by small V-T rates. Typical characteristic times for V-V, e-V and V-T processes in a N_2 discharge are given in Table 6.1 [11].

E/N (Vcm^2)	3×10^{-16}	6×10^{-16}
τ_{V-V}	5.5×10^{-4}	5.5×10^{-4}
τ_{e-V}	2×10^{-3}	1×10^{-3}
$\tau_{V-T}^{N_2}$	2.5×10^2	2.5×10^2

Table 6.1: Characteristic Relaxation times (τ) in N_2 plasmas ($n_e = 10^{11}cm^{-3}$, $T_g = 500$, $P_{N_2} = 5$ torr)

Since $\tau_{V-V} < \tau_{e-V} < \tau_{V-T}^{N_2}$, the vibrational quanta introduced by e-V energy exchange are distributed over the entire vibrational ladder of the molecule by the anharmonic V-V up-pumping mechanism. This leads to high degrees of vibrational non-equilibrium in the molecules. This high degree of vibrational non-equilibrium has a great impact on the EEDF because of strong collisional coupling between electrons

and vibrationally excited molecules (via $e + A_2(v) \rightarrow e^* + A_2(v - 1)$) and hence on the characteristics of the discharge.

This section describes the strategy that can be applied to study flowing molecular plasmas such as those in arcjet thrusters with molecular propellants like Nitrogen, Ammonia and Hydrazine. All heavy particles can be assumed to be at a single temperature T_h corresponding to the gas temperature. The electrons as discussed earlier, cannot be characterized by a single temperature, but by an electron energy distribution function. A spatially independent form of the Boltzmann equation describing the electron energies can be solved in a manner attempted by Nighan [4]. In studying such discharges, a judicious choice of the species and their internal levels that are modeled should be carefully made. Each internal level of a specie is then modeled as a separate chemical specie. This choice is extremely important as it serves to reduce the set governing equations and hence computing time. Such an effort would be a significant improvement over the work of Nighan, which does not include coupling with the flow field or Maxwell's equations. Before outlining this strategy, a brief discussion of electron kinetic analysis following reference [4] is described below.

The steady-state electron velocity distribution for a spatially uniform gas subjected to an electric field $\vec{E}$ is given by the well-known Boltzmann equation. The right-hand side of this equation denotes the rate of change of $f(\vec{v})$ due to electron collisions of all types.

$$\frac{-e\vec{E}}{m} \nabla_v f(\vec{v}) = \left(\frac{\delta f(\vec{v})}{\delta t} \right)_c \quad (6.1)$$

In the above equation $f(\vec{v})$ is the electron *velocity* distribution function. Since we are not interested in the direction of the velocities, the spatial dependence of

velocities is removed by integrating the velocity distribution function over the total solid angle. Note that f can still vary with position and time through v and $\delta f/\delta t$. Assuming the electron velocity function to be nearly spherically symmetric, $f(\vec{v})$ can be written as a sum of an isotropic function and a perturbation describing the anisotropy; as $f(\vec{v}) = f_0(v) + \vec{f}_1(v) \cdot (\vec{v}/v)$. Such a two-term expansion is valid when the directed velocity due to the field is small compared to the random thermal velocity. This ensures that the anisotropy of the distribution function. Using this two-term approximation for $f(\vec{v})$ in equation 6.1 yields a set of coupled equations for $f_0(v)$ and $\vec{f}_1(v)$ as follows.

Let $\vec{E}$ be the applied electric field with components E_x , E_y and E_z in the x,y and z directions. Let $\cos\theta_x$, $\cos\theta_y$ and $\cos\theta_z$ represent the direction cosines with these axes. The electron velocity distribution function depends only on the velocity $\vec{v}$ and the direction cosines. θ_x , θ_y and θ_z determine the direction between the velocity $\vec{v}$ and the individual axes. The distribution function in component form can be written as:

$$f(\vec{v}) = f_0(v) + \frac{v_x}{v} f_{1x}(v) + \frac{v_y}{v} f_{1y}(v) + \frac{v_z}{v} f_{1z}(v) \quad (6.2)$$

where $\vec{f}_1(v)$ has the components f_{1x} , f_{1y} and f_{1z} .

For clarity, only one of the components of equation 6.1 will be examined. Substituting equation 6.2 in equation 6.1,

$$a_x \frac{\partial}{\partial v_x} \left(f_0(v) + \frac{v_x}{v} f_{1x}(v) \right) = \left(\frac{\delta f(\vec{v})}{\delta t} \right)_c \quad (6.3)$$

where $a_x = -eE_x/m$.

The right hand side of the above equation can then be written as

$$\begin{aligned}
a_x \frac{\partial}{\partial v_x} \left(f_0(v) + \frac{v_x}{v} f_{1x}(v) \right) &= a_x \left[\frac{v_x}{v} \frac{\partial f_0}{\partial v} + \frac{f_1}{v} + \frac{v_x^2}{v} \frac{\partial}{\partial v} \left(\frac{f_1}{v} \right) \right], \\
&= a_x \left[\frac{v_x}{v} \frac{\partial f_0}{\partial v} + \frac{f_1}{v} + \frac{v_x^2}{v^2} \frac{\partial f_1}{\partial v} - \frac{v_x^2}{v^2} \left(\frac{f_1}{v} \right) \right], \\
&= a_x \left[\cos\theta_x \frac{\partial f_0}{\partial v} + \frac{f_1}{v} + \cos^2\theta_x \frac{\partial f_1}{\partial v} - \cos^2\theta_x \left(\frac{f_1}{v} \right) \right]
\end{aligned}$$

where $(\cos\theta_x = v_x/v)$.

Integrating the above equation over the solid angle and dividing by 4π gives an equation for f_0 ; Multiplying the above equation by $\cos\theta$ and integrating over the solid angle and multiplying the result with $3/4\pi$ gives an equation for f_{1x} . These equations are:

$$-a_x \left[\frac{f_1}{v} + \frac{1}{3} v \frac{\partial}{\partial v} \left(\frac{f_1}{v} \right) \right] = S_o$$

or

$$-\frac{a_x}{3v^2} \frac{\partial}{\partial v} (v^2 f_1) = S_o \quad (6.4)$$

$$-a_x \frac{\partial f_0}{\partial v} = \tilde{S}_1 \quad (6.5)$$

where

$$S_o = \frac{1}{4\pi} \int_{\omega} \left(\frac{\delta f(\vec{v})}{\delta t} \right)_c d\omega \quad (6.6)$$

and

$$S_1 = \frac{3}{4\pi} \int_{\omega} \left(\frac{\delta f(\vec{v})}{\delta t} \right)_c \cos\theta_x d\omega \quad (6.7)$$

This treatment can be generalised to include all the components of $f(\vec{v})$. The procedure is the same as that outlined above. $f_o(v)$ is obtained by integrating over all the velocity directions (i.e. integrating over the solid angle) and the three components of the anisotropic part can be obtained by averaging after multiplying by the direction

cosines of the angles between the velocity vector and each coordinate axis. These equations can then be written as:

$$\frac{-e\vec{E}}{3mv^2} \cdot \frac{d}{dv} [v^2 \vec{f}_1(v)] = S_o \quad (6.8)$$

$$\frac{-e\vec{E}}{m} \frac{df_0(v)}{dv} = \vec{S}_1 \quad (6.9)$$

where

$$S_o = \frac{1}{4\pi} \int_{\omega} \left(\frac{\delta f(\vec{v})}{\delta t} \right)_c d\omega \quad (6.10)$$

and

$$S_{1_k} = \frac{3}{4\pi} \int_{\omega} \left(\frac{\delta f(\vec{v})}{\delta t} \right)_c \cos\theta_k d\omega \quad (6.11)$$

where θ_k is the angle between the k^{th} axis and the velocity vector and the integration is carried out over the solid angles covering all the velocity directions. Assuming that electron-heavy particle momentum-transfer collisions play a major role in reducing the asymmetry in the distribution we have the following condition,

$$S_1 = - \sum \nu_{ej}(v) \vec{f}_1(v) \quad (6.12)$$

ν_{ej} is the electron momentum-transfer collision frequency for the j^{th} species. It is related to the number density and the momentum-transfer cross-section by the following expression:- $\nu_{ej} = N_j Q_{ej}(v) v$.

Using equations 6.9 and 6.12, with 6.8, an equation for the isotropic part of $f(\vec{v})$ can be obtained. This equation can be modified by the following transformation; $\epsilon = mv^2/2e$ and expressed in terms of ϵ as follows.

$$-\frac{E^2}{3} \frac{d}{d\epsilon} \left(\epsilon \frac{df_0}{d\epsilon} \left[\sum_j N_j Q_{ej}(\epsilon) \right]^{-1} \right) = S_o \quad (6.13)$$

This distribution function is normalized by:

$$\int_0^{\infty} \epsilon^{1/2} f_0(\epsilon) d\epsilon = 1 \quad (6.14)$$

Equation 6.13 is the electron energy distribution function, where ϵ is the average electron energy. Since most plasmas in engineering applications have average electron energies in the range of between 0.5-3.0 eV, only electron collisions resulting in vibrational and electronic excitation dominate electron-molecule energy exchange. Therefore the collision term in equation 6.13 can be written as:

$$S_o = \sum_{j,k} N_j [(\epsilon + \epsilon_{jk}) f(\epsilon + \epsilon_{jk}) Q_{jk}(\epsilon + \epsilon_{jk}) - \epsilon f(\epsilon) Q_{jk}(\epsilon)] \quad (6.15)$$

ϵ_{jk} is the energy loss (or gain) corresponding to the excitation or de-excitation of the k^{th} vibrational or electronic level of the j^{th} species of a neutral molecule due to electron impact. The above equation is a second-order ordinary differential equation that can be solved to obtain an expression for the EEDF.

In Nighan's approach the EEDF is obtained for prescribed values of E/n_T , however, the structure of the plasma model used in this work allows the equations describing f_o and f_1 to be solved in conjunction with the flow and Maxwell's equations yielding the electric field $\vec{E}$ and n_T , self-consistently. The variables E/n_T and δ_j can be obtained at each point in the computational domain by solving the flow, energy and species equations. The EEDF can then be obtained at each point in the computational domain, at each time-step. The EEDF thus obtained can be used in the evaluation of transport properties. Since there exists a strong coupling between these flow variables and the EEDF, the approach described above would be a reasonably accurate description of the flowing molecular plasma.

Direct solution of the EEDF with flow and Maxwell's equations has, to the best of the author's knowledge, never been attempted. Preliminary efforts in this direction have been reported by Belluci et al [62] using Euler equations and by Longo [63] using PIC Monte Carlo methods. The methodology outlined above allows a self-consistent computation of the EEDF together with Maxwell's equations for 2-D flows.

6.3 2-D Flow with Vibrational Non-Equilibrium

The above methodology can be applied to investigate the mechanisms whereby input electrical energy is consumed in arcjet thrusters. Knowledge of the EEDF and the relative importance of various electron-molecule collisions may provide an answer to recovering some of the frozen flow losses. A first step in this daunting task is the inclusion of vibrational non-equilibrium in a gas mixture flowing through a CD nozzle. In other words, the VT, VV and SRD terms would be included in the species equations as described in Chapter II. Quasi 1-D flows with vibrational non-equilibrium have been studied recently by Babu et. al [12] using the LBI scheme. Solution of the set of equations given in Chapter II (Eq. 2.13 - 2.19) without the inclusion of the electromagnetic equations and chemical reactions are explored in a preliminary way in this work.

Flow through a nozzle with a throat-exit area ratio of ≈ 100 has been studied. The gas stream consists of a 20 %CO, 80% Ar mixture. 15 vibrational levels of CO have included in the study. The boundary conditions are the same as those discussed in Chapter II. The geometry has been choosen so as to closely mimic the area-ratio and length as the geometry studied in Reference [12]. The stagnation temperature and pressure are also identical to those studied by Babu et. al. However, since

the geometry studied in reference [12] was rectangular in cross-section, whereas it is circular in this study, the slope of the diverging section (i.e. half angle of expansion) is different in these two cases.

The objectives of this study are as follows:

1. To lay the foundation for coupling the EEDF with the flow and electromagnetics in 2-D
2. To make preliminary comparisons between the results obtained from quasi 1-D calculations with 2-D simulations
3. To study the performance characteristics of such an effort in terms of computing time

6.4 Results

Figure 6.1 compares the population distribution of the vibrational levels at the centerline and at a point close to the wall at the exit plane with those predicted by Babu et. al [12]. Figure 6.2 shows the temperature distribution predicted by Babu et. al and the centerline and wall temperature in this work. The wall temperature is an important parameter in the study of such flows as the exit plane temperature depends on the specified value of the wall temperature.

Preliminary results show that the distribution is more V-V pumped in regions close to the wall as compared to the centerline, at the exit plane. This could be due to one of several reasons; it can be seen in Fig. 6.1 that the temperature along the centerline is higher than the wall temperature in regions close to the exit plane. These higher temperatures, tend make the population distribution less V-V pumped

Figure 6.1: Comparison of Normalized Vibrational Population Distribution with Quasi 1-D

Figure 6.2: Comparison of Axial Temperature Distribution with Quasi 1-D

as compared to the distribution in regions close to the wall. The low residence time of the gas stream in the nozzle tends to “preserve” this distribution. Figure. 6.1 also shows that the population distribution is less V-V pumped as compared to the quasi 1-D case. This is due to the higher exit plane temperatures predicted in the present work. Another possible reason for the near boltzmann distribution predicted for this geometry is the very mild half-angle of expansion. In the geometry studied by Babu et. al, the half-angle is 15 degrees whereas in this work it is about 2 degrees.

The computational effort required was also evaluated as a result of this study. A performance evaluation of the code with different grid sizes and vibrational levels is shown in Table 6.2.

Mflops	Grid size	Vibrational Levels	CPU Secs /timestep
95.22	100 X 25	16	10
165	100 X 25	40	42
125	40 X 50	25	13

Table 6.2: Performance Characteristics

It can be seen that for a case with one monatomic specie and 40 vibrational levels of a diatomic specie, a fully optimized code runs at a speed of 165 Mflops in the uniprocessor mode of the CRAY Y-MP. A single time-step takes 42 seconds of CPU time. The computing time would be higher for cases that consider vibrational levels of more than one diatomic specie and those which include the solution of Maxwell’s

equations and Boltzmann equation. This clearly indicates that one requires to parallelize the code so as to enable obtaining solutions to such systems of equations in a reasonable amount of time.

CHAPTER 7

SUMMARY AND RECOMMENDATIONS FOR FUTURE RESEARCH

7.1 Research Summary

The primary contributions of this work are:

- A High-Performance numerical model to study plasma and reacting flows in a variety of geometrical configurations and operating conditions has been developed.
- Chemical kinetics and electromagnetics have been self-consistently coupled to obtain steady-state solutions to a variety of plasma flow problems, *for the first time*.
- *For the first time*, the complete gaseous phase of a transferred plasma welding arc has been modeled from first principles.
- A detailed single temperature model describing a Hydrogen arcjet has been developed.
- The results of simulations both for a transferred plasma arc and the arcjet have been compared with available experimental results. Very good agreement with experimental results is obtained in both cases.

- The versatility of the LBI scheme in handling complex plasma and reacting flows has been demonstrated. It is important to point out that the LBI scheme was originally not developed with plasma and reacting flows in mind. This work has been the first to demonstrate the use of the LBI algorithm for complicated problems.
- A method to include the solution of the Boltzmann equation along with the equations describing a flowing plasma has been developed.
- The role of artificial dissipation in the stable time-marching of the governing equations has been addressed.

7.2 Recommendations for Future Research

7.2.1 Improvement of Present Model for Hydrogen Arcjets

The solution of the Boltzmann equation for electron energies and the governing equations describing flowing plasmas greatly increases the level of complexity and the computing time. The present single temperature model is capable of providing fairly accurate results in very reasonable amounts of CPU time. Simplicity and reduced computing time are the two main advantages of the present model. As discussed in Chapter V, the three main drawbacks with the present single temperature model are its inability to predict a constricted arc, the single-temperature assumption itself (which is not valid in the low density regions close to the exit plane or in the case of molecular discharges) and the adverse effects of artificial dissipation in the region of the arc. Modification of the present model to simulate a more realistic description of the arc would be advantageous from the vantage point of reducing programming

efforts and computing time. Such a model could serve as a design tool to predict the operating characteristics of electric discharges.

The diffuse nature of the arc predicted in Chapter V for the 1KW hydrogen arcjet could be a consequence of either the single temperature assumption, excess artificial dissipation in the constrictor region, or both. The effects of artificial dissipation on the solution can be studied by decomposing the present physical domain into two regions along the axial location corresponding to the exit of the constrictor. Thus, the plenum and the constrictor would comprise one region and the diverging section the other. The governing equations can then be solved in the two domains separately as in the case of the plasma welding arc described in Chapter V. Using an optimized dissipation model in the plenum and constrictor region, a converged solution can be obtained. Optimization can be sought by gradually reducing the values of μ_x and μ_r in the governing equations and studying their effects on stability and convergence. The values of all the dependent variables along the edge of the constrictor region (obtained by implicit extrapolation) can then be used as inlet conditions for the diverging section. Such a strategy has the virtue of isolating the effects of excessive artificial dissipation and its influence on the energy loading of the propellant. A two-temperature description of the plasma would be needed to better model exit plane conditions (especially of the temperature). There will be no changes in the operating conditions and the physical domain, though an additional energy equation to describe electron temperature would have to be added. This is analogous to replacing the EEDF with a single equation for the average energy of the electrons. All heavy particles would be at a single temperature (T_h) and the electrons at a different temperature (T_e). In low-pressure discharges, since $T_e > T_h$, it is likely that the predicted heavy particle

temperatures at the exit plane will be lower than those temperatures predicted by the single temperature model in this work. These modifications to the present single temperature model may simulate the constricted arc observed in experiments. Better prediction of flow-field variables is plausible if these modifications are made to the present single temperature model.

7.2.2 Flows in Plasma torches

The straight polarity mode of operation of the plasma torch has been investigated. Two different arc models were studied to evaluate their impact on the exit plane characteristics. Experimental measurements on the plasma torch [60] concluded that asymmetries in the electrode or orifice geometries likely result in the skewing of the plasma jet. These asymmetries may have arisen due to initial misalignment, operation of the pilot arc, deterioration of the electrode and orifice geometry during long operations. Correctly simulating such a plasma jet would require a 3-D simulation. However, such a study is very complicated and time-consuming.

The pilot arc needs to be included in the calculations in order to improve the existing VPPA torch model. The present approach solves Maxwell's equations using a single equation in terms of the magnetic induction B_θ . Specification of boundary conditions with such a formulation for the pilot and main arc would be far from trivial. Hence, inclusion of the pilot arc may require Maxwell's equation to be solved in terms of ϕ (the scalar potential) instead of the magnetic induction B_θ .

7.3 Inclusion of EEDF in modeling flowing plasmas

Preliminary studies have been performed on modeling flows involving vibrational kinetics in 2-D. To the best of this author's knowledge such an investigation has not

been published in the unclassified literature. An important consideration in such simulations is CPU time. It was clear from these studies that parallel computing techniques need to be invoked to solve such problems. Hence, any attempt to include Maxwell's equations and evaluation of the EEDF in simulating flowing plasmas would require parallelization of the existing code which is currently, designed and optimized for the uniprocessor mode on the CRAY Y-MP. The LBI scheme is very well-suited for parallel machines.

7.4 Improvements in Dissipation Models

The LBI scheme has been extended to model plasma and reacting flows in this work. This work has highlighted the need for more robust and versatile artificial dissipation models. At this point, artificial dissipation models are ad-hoc. The block-tridiagonal nature of the matrices resulting from the LBI method makes it difficult to derive a mathematical basis for the minimum amount of dissipation that needs to be added at each point to maintain stability. Hence, the dissipation models are problem-dependent. The effects of artificial dissipation are determined *a posteriori*. This process is time-consuming but necessary to ensure that the solution is not distorted due to the effects of dissipation. Hence, attempts must be made to develop global dissipation models that ensure stability, while maintaining the dissipation levels at a minimum in the converged solution.

Flowing plasmas are best described by multidimensional models which include non-equilibrium electron kinetics obtained by coupling the effects of a self-consistently computed electric-field, with vibrational kinetics. Parallel codes based on the LBI scheme with optimum amounts of dissipation would allow realistic simulations of a

wide variety of flowing plasmas. Such a detailed description of flowing plasmas will help clarify the underlying physics describing electrical discharges and contribute to improving many commercial applications.

BIBLIOGRAPHY

- [1] I. Langmuir. *Physical Review*, 33(954), 1929.
- [2] B. N. Chapman. *Glow Discharge Processes*. John Wiley & Sons, 1980.
- [3] C. E. Treanor, J. W. Rich and R. G. Rehm. *J. Chem. Phys*, 48:1798, 1968.
- [4] W. L. Nighan. Electron Energy Distributions and Collision Rates in Electrically Excited N_2 , CO and CO_2 . *Physical Review A*, 2(5):1989–2000, November 1970.
- [5] Panel on Opportunities in Plasma Science and Technology. *Plasma Science-From Fundamental Research to Technological Applications*. National Academy Press, 1995.
- [6] W. F. Hughes, and F. J. Young. *Electromagnetodynamics of Fluids*. John Wiley & Sons, NY, 1966.
- [7] E. S. Oran and J. P. Boris. *Numerical Simulation of Reactive Flow*. Elsevier, 1987.
- [8] S. Nakamura. *Applied Numerical Methods in C*. Prentice Hall, 1993.
- [9] M. Mitchner and C. H. Kruger, Jr. *Partially Ionized Gases*. John Wiley & Sons, 1973.
- [10] D. A. Anderson, J. C. Tannehill, and R. H. Pletcher. *Computational Fluid Mechanics and Heat Transfer*. Hemisphere Publishing, 1984.
- [11] M. Capitelli, editor. *Non-equilibrium Vibrational Kinetics*, volume 39 of *Topics in Current Physics*. Springer-Verlag, 1986.
- [12] V. Babu and V. V. Subramaniam. Numerical Solutions to Nozzle Flows with Vibrational Non-equilibrium. *Journal of Thermophysics & Heat Transfer*, 9(2):227–232, April-June 1995.
- [13] J. W. Rich et al. Strong Vibrational Non-equilibrium in Supersonic Nozzle Flows. *AIAA J.*, 31(1):119–128, 1993.

- [14] W. R. Briley and H. McDonald. *Journal of Computational Physics*, 24:372–397, 1977.
- [15] N. E. Todreas, and M. S. Kazimi. *Nuclear Systems I - Thermal-Hydraulic Fundamentals*. Taylor & Francis, 1990.
- [16] I. G. Currie. *Fundamental Mechanics of Fluids*. McGraw-Hill, 1974.
- [17] W. G. Vincenti and C. H. Kruger, Jr. *Introduction to Physical Gas Dynamics*. Kriger Publishing Company, FL, 1968.
- [18] G. W. Sutton and A. Sherman. *Engineering Magnetohydrodynamics*. McGraw-Hill, New York, 1965.
- [19] R. W. MacCormack. In *AIAA Paper 81-0110*, 1981.
- [20] R. M. Beam and R. F. Warming. *AIAA Journal*, 16(4):393–402, 1978.
- [21] R. D. Richtmeyer and K. W. Morton. *Difference Methods for Initial Value Problems*. Interscience Publishers, John-Wiley & Sons, 2nd edition, 1967.
- [22] E. Isaacson and H. B. Keller. *Analysis of Numerical Methods*. Wiley, New York, 1966.
- [23] W. F. Hansen and K. Clark. *Numerical Methods in Reactor Analysis*. Academic Press, 1964.
- [24] A. R. Mitchell. *Numerical Methods for Partial Differential Equations*. Barnes & Noble, New York, 1969.
- [25] J. F. Wendt, editor. *Computational fluid dynamics: An introduction*, chapter IX, pages 181–229. Springer-Verlag, 2nd edition, 1996.
- [26] V. Babu, S. M. Aithal and V. V. Subramaniam. Numerical Simulation of a H_2 Arcjet. *J. Propulsion & Power*, 12(6), Nov - Dec 1996.
- [27] S. M. Aithal, V. V. Subramaniam, and V. Babu. Effects of Arc Attachment on Arcjet Flows. In *Paper AIAA-96-3295 presented at the 32nd AIAA/ASME/SAE/ASEE Joint Propulsion Conference, July 1-3, 1996, Lake Buena Vista, FL*.
- [28] P. J. Roache. *Computational Fluid Dynamics*. Hermosa, Albuquerque, New Mexico, 1972.
- [29] J. S. Townsend. *Electricity in Gases*. Oxford University Press, 1915.
- [30] E. Pfender. *Gaseous Electronics*, chapter V. Academic Press, New York, 1978.

- [31] B. Glocker, H. O. Schrade, and P. C. Sleziona. Numerical Prediction of Arcjet Performance. In *paper AIAA-90-2612, 21st International Electric Propulsion Conference*, July 18-20, 1990, Orlando, Florida.
- [32] M. Auweter Kurtz, H. L. Kurtz, H. O. Schrade, and P. C. Sleziona. Numerical Modelling of the Flow Discharge in MPD Thrusters. *J. Propulsion & Power*, 5(1), Jan-Feb. 1989.
- [33] H. O. Schrade, and P. C. Sleziona. Basic Processes of Plasma Propulsion. Technical report, Interim Scientific Report, AFOSR-86-0337, July 1989.
- [34] G. W. Butler, B. A. Kashiwa, and D. Q. King. Numerical Modeling of Arcjet Performance. In *paper AIAA-90-1474, presented at the 21st International Electric Propulsion Conference*, July 18-20, 1990, Orlando, Florida.
- [35] D. Q. King, and G. W. Butler. Modeling and Measurement of N_2 Arcjet Performance. In *paper AIAA-90-2616, presented at the 21st International Electric Propulsion Conference*, July 18-20, 1990, Orlando, Florida.
- [36] R. P. Rhodes and D. Keefer. Numerical Modeling of an Arcjet. In *paper AIAA-90-2614, presented at the 21st International Electric Propulsion Conference*, July 18-20, 1990, Orlando, Florida.
- [37] S. A. Miller and M. Martinez-Sanchez. Multi-Fluid Nonequilibrium Simulation of Electrothermal Arcjets. In *paper AIAA-93-2101, presented at the 29th AIAA/SAE/ASME/ASEE Joint Propulsion Conference and Exhibit*, June 28-30, 1993, Monterey, California.
- [38] M. A. Cappelli et al. A Direct Comparison of Hydrogen Arcjet Thruster Properties to Model Predictions. In *paper IEPC-93-220 presented at the 23rd AIAA/AIDAA/DGLR/JSASS International Electric Propulsion Conference*, September 13-16, 1993, Seattle, Washington.
- [39] T. W. Megli, H. Krier and R. L. Burton. A plasmadynamics model for non-equilibrium processes in N_2/H_2 arcjets. In *In AIAA paper 95-1961, to appear in the J. of Thermophysics and Heat Transfer*, 1996.
- [40] T. W. Megli, J. Lu, H. Krier and R. L. Burton. Modeling Plasma Processes in 1 kw Hydrazine Arcjet Thrusters. In *In AIAA paper 96-2965 presented at the 32nd AIAA/ASME/SAE/ASEE Joint Propulsion Conference, July 1-3, 1996, Lake Buena Vista, FL*.
- [41] H. Okamoto, M. Nishida and K. Tanaka. Numerical Studies of the Flow Field of a low power DC Arcjet Thruster using Navier-Stokes Equations. In *paper IEPC-91-112, presented at the 22nd International Electric Propulsion Conference*, Oct, 1991, Viareggio, Italy.

- [42] J. A. Pobst, I. J. Wysonog and R. A. Spores. Laser-Induced Fluorescence of Ground State Hydrogen Atoms in an Arcjet Plume. In *paper IEPC-95-28 presented at the 24th International Electric Propulsion Conference*, Sept. 19-23, 1995, Moscow, Russia.
- [43] P. V. Storm and M. A. Cappelli. High Spectral Resolution Emission Study of a Low Power Hydrogen Arcjet Plume. In *paper AIAA-95-1960 presented at the 26th AIAA Plasmadynamics and Lasers Conference*, June 19-22, 1995, San Diego, California.
- [44] P. V. Storm and M. A. Cappelli. Fluorescence velocity measurements in the interior of a hydrogen arcjet nozzle. *AIAA J.*, 34(4):853-855, March 1996.
- [45] W. C. Gardiner, Jr. and G. B. Kistiakowsky. Thermal dissociation rate of hydrogen. *J. Chem. Phys.*, 35(5):1765-1769, November 1961.
- [46] R. K. Janev, et al. *Elementary Processes in Hydrogen-Helium Plasmas*. Springer-Verlag, NY, 1987.
- [47] G. W. Butler, I. D. Boyd, and M. A. Capelli. Non-equilibrium Flow Phenomena in Low Power Hydrogen Arcjets. In *Paper AIAA-95-2819 presented at the 31th AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit*, July 10-12, 1995, San Diego, California.
- [48] I. Boyd. Monte Carlo Simulation of Non-equilibrium Flow in Low Power Hydrogen Arcjets. In *Paper AIAA-96-2022 (Invited), presented at the 27th AIAA Fluid Dynamics Conference*, June 17-20, 1996, New Orleans, Louisiana.
- [49] W. D. Hayes and R. R. Probstein. *Hypersonic Flow Theory*. Academic Press, New York, 2nd edition, 1966.
- [50] W. A. Hargus, Jr. and M. A. Cappelli. Mass Flux Measurements in the Plume of a Low Power Arcjet Nozzle. In *paper AIAA 96-3190, presented at the 32nd AIAA/ASME/SAE/ASEE, Joint Propulsion Conference*, July 1-3, 1996, Lake Buena Vista, FL.
- [51] J. Dowden, P. Kapadia and B. Fenn. Space charge in plasma arc welding and cutting. *J. Phys. D: Appl. Phys.*, 26, 1993.
- [52] A. C. Nunes et al. The Variable Polarity Plasma Arc Welding Process: Its application to the Space Shuttle External Tank - First Interim Report. Technical report, NASA Technical Memorandum NASA TM-82532, June 1983.
- [53] J. McKelliget, J. Szekely, M. Vardelle and P. Fauchais. *Plasma Chem. Plasma Process.*, 2, 1992.

- [54] A. H. Dilawari and J. Szekely. *Plasma Chem. Plasma Process.*, 7, 1987.
- [55] Y. C. Lee and E. Pfender. Particle dynamics and particle heat and mass transfer in thermal plasmas. Part III. Thermal plasma jet reactors and multiparticle injection. *Plasma Chem. Plasma Process.*, 7(1), 1987.
- [56] D. A. Scott, P. Kovitya and G. N. Haddad. Temperatures in the plume of a DC plasma torch. *J. Appl. Phys.*, 66(11), December 1989.
- [57] R. Westhoff and J. Szekely. A model of fluid, heat flow and electromagnetic phenomena in a nontransferred arc plasma torch. *J. Appl. Phys.*, 70(7):3455–3466, October 1991.
- [58] A. B. Murphy and P. Kovitya. Mathematical model and laser-scattering temperature measurements of a direct-current plasma torch discharging in air. *J. Appl. Phys.*, 73(10), May 1993.
- [59] J. R. Fincke, S. C. Snyder and W. D. Swank. Comparison of enthalpy probe and laser light scattering measurement of thermal plasma temperatures and velocities. *Rev. Sci. Instrum.*, 64(3), March 1993.
- [60] J. M. Pagan. Master's thesis, The Ohio State University, Columbus, OH, June 1996.
- [61] H. Schlichting. *Boundary Layer Theory*. McGraw-Hill Book Company, 7th edition, 1970.
- [62] V. Belluci et al. Vibrational kinetics for numerical simulation of thermal non-equilibrium flows. In M. Capitelli, editor, *Molecular Physics and Hypersonic Flows*. Kluwer Academic Publishers, Dordrecht, 1996.
- [63] S. Longo. Self consistent modeling of free electron kinetics. In M. Capitelli, editor, *Molecular Physics and Hypersonic Flows*. Kluwer Academic Publishers, Dordrecht, 1996.