Cascade arc studies of nonequilibrium hydrogen/nitrogen plasmas

Trevor Michael Moeller

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Dennis Keefer, Major Professor

We have read this dissertation and recommend its acceptance:

Frank Collins, Ahmad Vakili, Roy Schulz

Accepted for the Council:

Carolyn R. Hodges

Vice Provost and Dean of the Graduate School

(Original signatures are on file with official student records.)
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Dr. Dennis Keefer, Major Professor

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Accepted for the Council:

[Signatures]

Associate Vice Chancellor
and Dean of The Graduate School
CASCADE ARC STUDIES OF NONEQUILIBRIUM
HYDROGEN/NITROGEN PLASMAS

A Dissertation
Presented for the
Doctor of Philosophy
Degree
The University of Tennessee, Knoxville

Trevor Michael Moeller
May 1998
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ABSTRACT

A cascade arc facility was developed to study the characteristics of nonequilibrium plasma propellants for electric propulsion applications. The cascade arc was operated with 50 A hydrogen arcs at 2.0 and 6.0 psi. Spatially resolved spectral emission data were collected using a two dimensional Optical Multichannel Analyzer (OMA). Electron density was determined by fitting theoretical line profiles to experimentally measured Abel inverted emission line profiles. Radial distributions of plasma temperature were estimated from Boltzmann plots of spectral line intensity. The measured electron densities and plasma temperatures were compared to values predicted by nonequilibrium cascade arc simulations using the UTSI Cascade Arc Plasma Simulation (CAPS) code. The simulations underpredicted the peak experimental electron densities by as much as an order of magnitude and over predicted peak plasma temperatures by as much as a factor of 2.5. The experimental electric field has been accurately predicted by varying chemical kinetics in the CAPS code. Kinetic models developed at the University of Illinois gave the best agreement with the Cascade Arc measurements for hydrogen. Electron number density profiles for simulated ammonia and hydrazine were also obtained at pressures of 2.0, 6.0, and 10.0 psi. These hydrogen/nitrogen mixture data can be used in comparisons with a hydrogen/nitrogen version of the CAPS code expected to be developed in the future.
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CHAPTER 1

INTRODUCTION

Arcjets offer significant advantages for satellite station keeping and maneuvering, since their specific impulse can be more than twice that of conventional resistojet or chemical thrusters commonly used for these missions. Four commercial satellites using these new arcjet thrusters for orbit maintenance are already in use [1]. Current arcjet performance, however, is far below the limits of an ideal arcjet, leaving room for significant improvements. Computational codes can be used to guide refinements in the basic arcjet configuration which would lead to more uniform radial temperature profiles, and a number of arcjet codes have been developed for this purpose [2-5]. However, it is now clear that there are important nonequilibrium processes in the propellant plasma which must be understood before adequate physical models can be constructed for use in these computational codes. A cascade arc facility has been constructed at UTSA which permits measurements of nonequilibrium transport properties to be made on a controlled nonequilibrium propellant plasma to guide development of the physical models required for further development of the computational codes. The work presented in this dissertation addresses the task of the development of a better finite rate chemical kinetics model and a nonequilibrium transport property model for a hydrogen plasma for use in arcjet simulation codes.
1.1 What Is an Arcjet?

Arcjets are electrothermal thrusters for use in space. They evolved from the monopropellant thrusters originally utilized for satellite station keeping. These monopropellant thrusters expand a propellant gas out of a nozzle to produce thrust at a specific impulse, $I_{sp}$, of 240 seconds [6]. To increase $I_{sp}$ and reduce the amount of fuel required for station keeping over a satellite's lifetime, a resistor was added to the monopropellant thruster concept and the resistojet was born. By heating the propellant gas with the electrical power dissipated in the resistor before the propellant expands out the nozzle, a typical resistojet's $I_{sp}$ becomes 300 seconds [6]. To increase the $I_{sp}$ of the resistojet even further, the gas must be heated to a higher temperature than is obtained with the resistor. To accomplish this, the resistor was replaced with an electric arc; the arcjet with an $I_{sp}$ of 600 seconds [6] is the result.

Arcjets are comprised of three major components—a cathode, an electrode, and an insulator (Figure 1.1). The anode forms the constrictor (throat of the arcjet), nozzle, and part of the plenum upstream of the constrictor. The cathode is a cylindrical rod with a pointed tip and is usually positioned with its tip protruding part way into the constrictor. The closest distance between the cathode and anode is called the anode-cathode gap. The cathode is centered in the axially symmetric anode via the insulator.

The arcjet works by heating the propellant to a plasma as it passes through an electric arc between the cathode and anode. Under proper operating conditions, the arc attaches to the anode in the nozzle region. When the propellant exits the constrictor, its heat energy is converted into directed kinetic energy as it expands out the nozzle, and thrust is produced.
Because the arc wants to minimize its path length, the point of attachment can be in the constrictor. This operation mode results in excessive temperatures in the constrictor that cause ablation damage. Mass flow rate determines the attachment point and is adjusted to prevent this situation. The required mass flow rate depends on the arc voltage. The flow of current between the cathode and anode induces an azimuthal magnetic field which results in a force that causes slight axial acceleration and radial compression. The radial compression pinches the arc and can lead to arc instability; poor arcjet performance can result. Two methods have been used to help stabilize the arc. The first method involves controlling the arc with an applied magnetic field [6]. A more common approach is to introduce the propellant with an azimuthal velocity component. Hence, the propellant has a helical motion, or swirl, as it moves through the arcjet. The swirling propellant maintains a cold boundary layer in the constrictor and stabilizes the arc. The electrical conductivity of the propellant
in this boundary layer is lowered; therefore, a higher arc voltage is required for proper arcjet operation.

Energy is put into the flow through the free electrons. Electrons emitted from the cathode are accelerated in the electric field between the anode and cathode. Part of the electron kinetic energy is transferred to the heavy particles when collisions occur—Ohmic heating. Given enough collisions, the temperature of the electrons and heavy particles will equilibrate (thermal equilibrium). Thermal equilibrium is only attained in regions in the flow where particle number densities are high enough for a sufficient number of collisions. To attain chemical equilibrium, the time scale of the chemical reactions taking place must be much smaller than the time required for the particles to traverse the area of interest. In the arcjet, particle resident time is smaller than chemical reaction times. Number densities vary between regions in the flow. Densities are high enough in regions upstream of the constrictor for these areas to be considered in thermal equilibrium; the region upstream of the constrictor is the only place where chemical equilibrium is reached. The constrictor and nozzle have not equilibrated because of the low number densities that are a result of the expansion of the flow and the high gas velocity that results in a residence times too short for the chemical reactions to reach completion.

The efficiency of an arcjet is defined as the ratio of the power in propellant kinetic energy to the electric power input. Depending on the power and type of propellant used, efficiencies range from about 30 percent for propellants with large molecular weights to about 40 percent for hydrogen [6]. Therefore, 30 to 40 percent of the power input is converted to thrust; the rest of the energy is lost. Arcjets have several loss mechanisms. Some of the energy is dissipated in the anode and cathode due to electrical resistance. Conduction losses can occur at the walls if the gas
temperature is greater than the boundary temperature—the opposite temperature gradient will result in energy addition to the flow. Recombination losses occur when the atoms, ions, and electrons do not have enough time to recombine as they are accelerating and cooling in the nozzle. The flow is not in equilibrium when recombination losses are present. Optically thin radiation which passes from the hot, central core of the flow to the walls is another loss mechanism [7]. This radiation energy results in heating the arcjet walls. Because of viscous dissipation, some directed kinetic energy is converted back into heat energy—another loss mechanism. The excess energy must ultimately be rejected from the system through radiation cooling.

The power per unit volume input to the propellant due to Ohmic heating is

$$P_{\text{Ohmic}} = \sigma \cdot E^2$$

(1.1)

where $E$ is the electric field strength and $\sigma$ is the electrical conductivity. Most of the power input to the propellant flow occurs near the centerline of the constrictor where the electrical conductivity is highest. This region of the flow also has the highest temperature and, therefore, has the lowest density. As a result, most of the energy input to the system is added to the portion of the propellant that has the lowest density. Most of the propellant mass is flowing in regions around the arc where little energy addition occurs. Through species diffusion and chemical and radiation transport, some of the energy in the low density core diffuses into the cold, dense surrounding gas. This energy transport is limited by the short time that the high velocity gas is in the constrictor. Therefore, the radial temperature profile in the arcjet is determined by a complicated balance of Ohmic heating with thermal
diffusion, radiation transport, and chemical transport. Future improvements in arcjet performance require that a larger fraction of the propellant passing through the constrictor be heated to high temperatures resulting in a much flatter temperature profile and greater $I_{sp}$. This may be accomplished by changing the geometry of the arcjet or seeding the propellant to change energy transport properties to transport more energy to the colder, denser gas around the arc.

It is believed that arcjet performance can be improved through geometric changes to the general arcjet configuration. Currently, this requires that a design change based on an educated guess be made to the arcjet. To test the effects of this change, the new parts must be machined, the arcjet must be fabricated, and the performance of the new thruster must be measured in a vacuum facility. This process is repeated many times until the necessary improvements are obtained. Optimization of the arcjet using this approach is very time consuming and expensive. Much could be gained from an arcjet computer simulation code that could be used to accurately predict the changes in performance as a result of design changes. This would allow the optimization to be faster and less expensive because the number of times a prototype arcjet would need to be constructed and tested could be greatly reduced.

1.2 Arcjet Computer Simulation Codes

A number of two-dimensional, axisymmetric arcjet simulation codes have been developed to simulate arcjet thrusters [2-5]. The earlier of these codes assumed local thermodynamic equilibrium (LTE). The physical models are greatly simplified by this assumption since there is only one energy equation (thermal equilibrium) and plasma species are determined by chemical equilibrium. These assumptions, however, lead to
unrealistically low electrical conductivity in cold regions of the flow where the arc attaches to the nozzle [2]. An *ad hoc* modification to artificially raise the electrical conductivity in this region has been used [2] to obtain realistic simulations of the arcjet. Simulations of hydrogen arcjets using these models predicted well the trends seen in data from arcjet experiments [7]. However, simulations comparing water-cooled and radiation-cooled hydrogen arcjets demonstrated the inadequacy of the equilibrium arcjet assumption [8].

Later codes assuming both thermal and chemical nonequilibrium removed the artificial increase to electrical conductivity necessary in the codes assuming LTE. Simulations using these models have better agreement with experiment [2,4,5]. With the chemical nonequilibrium assumption used in these codes, plasma constituents are determined by species diffusion and chemical kinetics. The electrical conductivity in the cold region near the arcjet wall is larger than that predicted by the LTE models because the electron population is greatly increased by diffusion from the hot core. To adequately predict electrical conductivity, accurate diffusion coefficients and chemical kinetic rates, especially those associated with electrons, must be well known. Thermal nonequilibrium assumes two different Maxwellian distribution functions for the electrons and heavy particles at different temperatures; this results in two energy equations, one for the heavy particles and one for the electrons. Electrical energy is absorbed into the electrons and transferred to the heavy particles through collisions. Therefore, the electron temperature will exceed heavy particle temperature in the hot core where energy is being absorbed [9]. In cold regions near the nozzle wall, little electrical energy is input. Inelastic collisions with molecular species in these cold regions can lower electron temperature below heavy particle temperature. Calculating the transport properties for nonequilibrium reacting plasmas of this type is
complex and requires detailed knowledge of species concentrations along with electron-molecule collision cross-sections over a range of low energies (less than 1.5 eV) [9].

The thermal and chemical nonequilibrium codes predict trends in arcjet performance quite well but are not accurate enough to determine effects of slight design changes on performance. Comparison of simulation results with experimental data make it clear that physical models of nonequilibrium processes in a plasma must be verified and refined before the effects of small changes in arcjet geometry will be accurately predicted [2,8]. Both the finite rate chemical kinetic models and nonequilibrium transport properties need to be improved before the energy transport in the computer simulation can properly predict experimental results.

1.3 Nonequilibrium Transport Properties and Finite Rate Chemical Kinetics

Plasma models based on local thermodynamic equilibrium and chemical equilibrium lead to significant errors when modeling nonequilibrium plasmas. This is certainly true in the modeling of arcjet thrusters. Accurate transport property and chemistry calculations are essential to gas dynamic and heat transfer analyses in the arcjet problem. Theoretical nonequilibrium models based on the Collisional-Radiative (CR) model are generally accepted as the proper means to calculate nonequilibrium plasma properties [10-12]. The CR method models an atom or ion as a ground state, its electronic excited states, and the next higher ion or continuum, whichever the case may be [12]. The CR model incorporates both collisional and radiative processes that lead to transitions between these states and ultimately defines the composition of the plasma under consideration. Theoretical finite rate chemical kinetic models can be
developed from the results of CR modeling [12]. Since the occurrence of a collision depends on the collision cross-section associated with the interaction, CR modeling and CR based chemical kinetics depend on both theoretical and experimentally measured collision cross-sections.

Theoretical nonequilibrium transport properties also depend on collision cross-sections of the particle interactions in a plasma. For nonequilibrium plasmas, solution methods of the Boltzmann equation--BBGKY, Chapman-Eskog [11,13,14]--express the transport properties as functions of the plasma composition and intermolecular or interatomic potentials.

1.3.1 Determination of Nonequilibrium Transport Properties and Finite Rate Chemical Kinetics Using a Cascade Arc.

Better transport property and chemical kinetics models are needed before arcjet computer simulation codes can be improved. These models can be developed by comparing spectroscopic data from a cascade arc and a computer simulation of the cascade. Discrepancies between the experimental data and simulation results can guide refinement of the nonequilibrium models.

Maecker described the first cascade arc [15]. The cascade arc has cylindrical symmetry, well defined boundary conditions, and is capable of high power energy densities. Therefore, it is the method of choice for the measurement of transport properties of high temperature gases, including thermal conductivity, electrical conductivity, and radiation transport [16]. This cascade arc, also referred to as the wall stabilized arc, has been widely used to determine experimental values for transport properties for many gases since the 1960's. These data were obtained for
the validation of transport property models. Because it is easy to use and provides stable arcs, argon was used in a majority of the cascade arc experiments. Argon was used in tests with pressures ranging from a fraction of an atmosphere to hundreds of atmospheres, and over a temperature range from 9000 K to 25,000 K [16-43]. Other gases such as nitrogen [22,42,44-48,53], hydrogen [22,28,44], and air mixtures [49-51] have been tested over the same temperature regime as argon, but over a much more restricted pressure range.

1.3.2 What Is a Cascade Arc?

A cascade arc apparatus has a geometry similar to that of the constrictor in an arcjet, and a cascade arc can be run under conditions that produce nonequilibrium plasmas that are similar to those in an arcjet. The cascade arc apparatus is comprised of three sections, an anode, a cathode, and a constrictor. The arc that develops between the electrodes is stabilized in the constrictor separating them. A schematic of the UTSI Cascade Arc Facility appears in Figure 1.2. The constrictor section is comprised of a stack of individually water-cooled copper plates separated by electrical insulators. When stacked together, a central hole in the copper plates forms the constrictor. An electrode is located at each end of the constrictor. When voltage is applied across the electrodes, electrons flow from the cathode, through the constrictor, and are absorbed into the anode. The electrons do not travel through the copper plates because the insulators between the plates raise this current path's resistance above the resistance of the test gas in the constrictor; thus, the plates constrict and stabilize the arc. The central copper plate is a modified plate that has
windows to allow optical access to the plasma gas. Optical measurements of the plasma radiation allow the nonequilibrium plasma properties to be determined and compared to computer simulations. A detailed discussion of the cascade arc facility and its components is given in Chapter 3.

1.3.3 Reasons For Utilizing a Cascade Arc Rather Than an Arcjet.

Some of the most important chemical and transport processes in an arcjet arc, e.g. radial species diffusion and recombination, occur on time scales that are comparable to the convective times in an arcjet. This fast convection produces the strong axial gradients found in an arcjet plasma. Therefore, the plasma conditions at a given point in an arcjet depend strongly on the previous history of the plasma passing through that point. Comparison of code predictions with measurements in this case requires that the entire upstream flow field be accurately predicted. Differences
between measured and predicted quantities could be due to inaccuracies in the models at any point upstream of the measurement location. This makes it very difficult to assess which model mechanisms or rates should be altered to improve the code.

Cascade arcs have long been used as a means to measure the fundamental atomic constants and transport properties of high temperature gases [52]. The cascade arc has a diameter similar to that of an arcjet constrictor but the flow velocity is much smaller and the length of the arc is tens of diameters as compared to one diameter in an arcjet. This produces an arc with similar properties to an arcjet but with negligible axial gradients. The radial temperature profiles in the cascade arc are controlled primarily by diffusive transport properties rather than convection. In the cascade arc, where there are no significant axial gradients, the nonequilibrium plasma parameters are determined by a balance between radial diffusion and chemical reactions and an axially constant but radially dependent energy input. The plasma properties depend on the local conditions at the measurement station rather than a complex convolution of all the conditions upstream of the point of measurement. Differences observed between code predictions and measured quantities are more easily related to specific reactions or diffusion rates which must be modified to improve the code models.

The arc in an arcjet is confined within a constrictor/nozzle/anode made of tungsten. Accurate radial spatial resolution of the optical measurements is required for comparison with code predictions. Emission measurements require Abel inversion to obtain this spatial resolution, and accurate Abel inversion requires axial symmetry of the arc. It is difficult to obtain optical access through the typical large diameter tungsten piece which forms the arcjet constrictor/nozzle/anode. Some optical observations of an arcjet arc have been made through holes drilled into the tungsten
constrictor region [53]. However, this creates an opening at one azimuthal location and axial symmetry of the arc becomes compromised. Thus, the data cannot be Abel inverted with complete confidence. It is also difficult to provide the optical access required for accurate absolute optical calibration. In the cascade arc the optical access can be made symmetric, preserving symmetry of the arc, and adequate solid angles are available to provide good absolute calibrations. Accurate optical measurements of the radial profiles, together with analysis based on an appropriate one-dimensional computational code, permit validation of the chemical kinetics and diffusive transport models and provide a basis for the development of physical models needed for the arcjet codes being developed.

1.4 Objective of Dissertation

The primary objective of this dissertation is to use optical measurements of nonequilibrium hydrogen cascade arc plasmas to guide the development of better finite rate chemistry models and nonequilibrium transport property models for use in arcjet thruster codes. Comparisons of the nonequilibrium hydrogen arc properties measured in the cascade arc with computer simulations of the cascade arc provide guidelines for adjusting both chemical kinetics and nonequilibrium transport property models. A secondary objective of this dissertation is to provide nonequilibrium plasma property data for simulated mixtures of ammonia and hydrazine.
1.5 Organization of Dissertation

Chapter 2 contains the theory and background of the Cascade Arc Plasma Simulation (CAPS) Code. The details of the transport property calculations and finite rate chemical kinetics calculations are also presented in this chapter. A description of the UTSI Cascade Arc Facility is given in Chapter 3. The design, machining, and fabrication of the facility components will be discussed in detail. The procedure used in the acquisition of data will be presented as well. Results from the numerical simulations are presented in Chapter 4, and the experimental data analysis is discussed in Chapter 5. A comparison of numerical results with computer simulations is presented in Chapter 6, and the physical models in the computer code are evaluated. Chapter 7 contains conclusions and recommendations for future work.
CHAPTER 2

THE UTSI CASCADE ARC PLASMA SIMULATION (CAPS) CODE

The equilibrium and nonequilibrium UTSI arcjet computer codes have been modified into pseudo one-dimensional equilibrium and nonequilibrium cascade arc computer codes [54] for predicting the radial distribution of arc conditions. At present these codes model a $H_2$, $H$, $H^+$, $e$ hydrogen system. Both codes include species diffusion and radiation transport. The nonequilibrium version has a two-temperature model for heavy species and electrons and a finite rate chemistry kinetics model. In both codes it is assumed that the radial pressure gradient is zero, the radial and azimuthal velocities are zero, and the radial current density is zero. It is also assumed that species concentrations do not vary axially. The required mass flow is assured by adjustment of velocity levels. The consequence of these assumptions is that species production and diffusion are locally balanced and total production is balanced by wall losses for the axial momentum, energy, electron energy, and species.

2.1 The Numeric Model and Governing Equations

The algorithm for the solution of the governing equations in the CAPS code is the same as that used in the UTSI arcjet simulation code [54]; however, the CAPS code assumptions mentioned above greatly simplify the governing equations in the arcjet code. The simplified governing equations are discussed in this section. The algorithm for the CAPS code is a Navier-Stokes solver based on the SIMPLE (Semi-
implicit Pressure Linked Equation) algorithm developed by Gosman and Pun [55] and modified by Rhie [56] to accommodate both supersonic and subsonic flow. Jeng [8, 57] and Rhodes [58] incorporated a magnetic field equation coupled with heat release to study laser heat addition and radio frequency heating of a plasma, respectively. The code is formulated to solve the steady-state Navier-Stokes equations. The governing equations in the code are solved in a transformed coordinate where the original, non-orthogonal, axially symmetric grid is mapped to a grid of unit squares [59]. Even though the UTSI cascade arc could be simulated using a one-dimensional code, the CAPS code calculations are performed on a two-dimensional grid. Assumptions in the code specify the radial velocity and radial current density to be zero. The radial pressure gradient is also specified to be zero. The axial velocity and pressure are, however, allowed to vary axially.

The computation grid representing the UTSI Cascade Arc is shown in Figure 2.1. The axial dimension is along the abscissa and the radial dimension is along the ordinate. The grid point density increases near the wall to aid code convergence in regions where radial gradients can be large. The CAPS code uses the program control and array structure used in the UTSI arcjet simulation code. As a result, the CAPS code computation grid requires an axial dimension. However, this allows axial variations in pressure and velocity to be simulated, and allows the confirmation of negligible axial gradients in the cascade arc plasma. The conservation equations are solved for grid cells in the transformed computation grid (see Figure 2.2). Data from the UTSI cascade arc are compared with simulations results in the second column of grid cells.
Figure 2.1 Computation grid (in spatial coordinates) used in the CAPS code simulations.
Figure 2.2 Computation cells surrounding points in a transformed computation grid. There are $N$ grid points and $N-1$ cells in the radial direction and four grid points and three cells in the axial direction.
The SIMPLE algorithm used in the CAPS code is a solver for equations of the form:

\[ \nabla \cdot \rho \bar{v} \phi = \nabla \cdot \Gamma \phi \nabla \phi + S \quad (2.1) \]

where \( \phi \) is a dummy variable representing the axial velocity (u), the static enthalpy (H), the pressure (p), the electron temperature (\( T_e \) for nonequilibrium), or species concentrations (\( \alpha_i \) for nonequilibrium). \( \Gamma \) represents the transport coefficient appropriate for each variable. Any terms which cannot be put into a convective or diffusive form are added to the source term, S. The transformation of the grid coordinates into a grid of unit squares results in mixed derivatives from diffusive terms that are also added to S [54]. Second order accurate finite difference representations are used to represent equation (2.1) for the variable under consideration at each point in the computation grid. Written in matrix form, these coupled equations result in a tri-diagonal matrix that is solved using a tri-diagonal solver. Equation (2.1) is solved sequentially for each of the dependent variables using under-relaxation. Updated values of the dependent variables are used when they are available, and old values are used when the variables have yet to be updated. The process of solving equation (2.1) for each of the dependent variables is repeated until the sum of all of the residual errors has been reduced to a small value [54]. At this point the numerical solution to the problem is no longer changing significantly.
2.1.1 Equilibrium/Nonequilibrium Momentum Equation

The form of the momentum conservation equation is the same for both the equilibrium and nonequilibrium cases. The axial velocities are obtained from the axial momentum equation for steady, axially symmetric flow [59]. The momentum equation, in vector form, is [2]

\[ \nabla \cdot \rho \vec{v} \cdot \nabla = -\nabla p + \nabla \cdot \tau + \vec{J} \times \vec{B} \]  \hspace{1cm} (2.2)

where \( \tau \) is the viscous stress tensor, \( \rho \) is the density, \( \vec{v} \) is the velocity of the gas (\( \vec{v} \) is equal to the axial velocity, \( u \)), \( p \) is the pressure, \( \vec{J} \) is the current density which only has an axial component \( (J_x) \), and \( \vec{B} \) is the magnetic field which only has an azimuthal component \( (B_\theta) \). The effects of the CAPS code assumptions on the momentum equation are easier to interpret when the equation is written in cylindrical coordinates.

The axial momentum equation in cylindrical coordinates is:

\[
\frac{1}{r} \frac{\partial}{\partial r} \left( \rho u^2 \right) + \frac{1}{r} \frac{\partial}{\partial r} (\rho \mu u v) = \frac{4}{3} \frac{\partial}{\partial x} \left( \mu \frac{\partial u}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( \mu \frac{\partial u}{\partial r} \right) - \frac{\partial}{\partial x} \left( \mu \frac{v}{r} \right) - \frac{2}{3r} \frac{\partial}{\partial x} (\mu v) + \frac{1}{r} \frac{\partial}{\partial r} \left( \mu \frac{v}{r} \right) - \frac{\partial p}{\partial x} + J_x B_\theta
\]  \hspace{1cm} (2.3)

where the viscosity, \( \mu \), is discussed in Section 2.4.2. The Lorentz body force term, \( \vec{J} \times \vec{B} \) or \( (J_x B_\theta) \), is zero because of assumptions in the code. Since the current has only an axial component and the magnetic field only has an azimuthal component, the cross product of \( \vec{J} \) and \( \vec{B} \) is in the radial direction. The flow in the cascade is assumed to be
axial; therefore, the Lorentz force in the radial direction has no effect on the momentum equation (only the axial momentum equation is solved in this problem). Therefore, the simplified momentum equation solved in the CAPS code is

\[
\frac{\partial}{\partial x} \left( \rho u^2 \right) = \frac{4}{3} \frac{\partial}{\partial x} \left( \mu \frac{\partial u}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( r \mu \frac{\partial u}{\partial r} \right) - \frac{\partial p}{\partial x} \tag{2.4}
\]

As mentioned above, the momentum equation is the same for both the equilibrium and the nonequilibrium versions of the code. The density, however, is calculated differently for the equilibrium and nonequilibrium versions. The equilibrium density is given by [54]

\[
\rho = \frac{pM}{RT} \tag{2.5}
\]

where

\begin{align*}
M & = \text{the molecular weight of the mixture} \\
R & = \text{the universal gas constant} \\
T & = \text{the gas temperature}
\end{align*}

The nonequilibrium density is given by [54]

\[
\rho = \frac{pM}{R \left[ T_h - (T_e - T_h) x_e \right]} \tag{2.6}
\]

where

\begin{align*}
T_h & = \text{the temperature of the heavy particles} \\
T_e & = \text{the temperature of the electrons} \\
x_e & = \text{the electron mole fraction}
\end{align*}
The addition of the mass continuity equation, $\nabla \cdot (\rho u) = 0$, allows the pressure to be calculated [2]. Because the mass flow rate in the cascade arc is very small, the axial velocities realized in the constrictor channel are also very small (approximately 10 m/s). These low velocities result in axial pressure gradients that do not significantly affect simulation results.

### 2.1.2 Equilibrium Energy Equation

The equilibrium CAPS code assumes local thermodynamic equilibrium (LTE). This assumption implies that the temperature of all of the particles in the gas is the same. Therefore, only one energy equation is necessary to describe a plasma in LTE. The static enthalpy, $H$, is obtained from the following energy equation which includes ohmic heating, radiation loss, and viscous dissipation [2].

$$
\nabla \cdot \rho \mathbf{v} H = \nabla \cdot \left( \frac{k}{C_p} \nabla H + \Phi + q_i - q_r + \mathbf{v} \cdot \nabla p \right)
$$

(2.7)

where

$$
\Phi = \text{viscous dissipation}
$$

(2.8)

and

$$
H = \text{mixture static enthalpy} = \sum \alpha_i h_i
$$

$h_i = \text{molar specific enthalpy of constituent 'i'}$

$C_p = \text{mixture specific heat} = \sum \alpha_i C_p$

$\alpha_i = \text{concentration of plasma constituent 'i'}$
$c_p$ = molar specific heat at constant pressure

$k$ = thermal conductivity

$q_i$ = ohmic heating = $J_x^2/\sigma$

$q_r$ = loss due to optically thin radiation

$r$ = radius

$\mu$ = viscosity

$p$ = pressure

$\bar{v}$ = mixture velocity.

$\rho$ = gas density.

The calculation of the thermodynamic properties and equilibrium transport properties will be discussed in Sections 2.4 and 2.5.

2.1.3 Nonequilibrium Energy Equation

Several choices are available for the form of the two energy equations necessary to describe a two-temperature nonequilibrium plasma. In this work, energy equations for the electron energy and the static energy of the whole mixture are used. These equations were chosen because the form of the energy balance for the whole mixture is the same as that for the equilibrium case [54].

Because the LTE assumption is relaxed in the nonequilibrium CAPS code, the temperature of the electrons is not necessarily equal to the temperature of the heavy particles. The energy distribution of the heavy particles and the electrons are assumed to be Boltzmann distributions at the heavy particle temperature and electron
temperature, respectively. Therefore, the energy in the system must be represented by two energy equations. The equation for the mixture enthalpy, $H$, is [54]

\[
\nabla \cdot \rho \nabla H = \\
= \nabla \cdot \left[ \frac{k}{C_{p_s}} \nabla H + \left( \rho D - \frac{k}{C_{p_s}} \right) \sum_i h_i \nabla \alpha \right.

\left. - k \alpha_e \frac{C_{p_s}}{C_{p_e}} \nabla T_e \right] \\
\]

(2.9)

\[+ \Phi + q_i - q_f + \nabla \cdot \nabla p \]

where

- $H = \text{mixture static enthalpy} = \sum \alpha_i h_i$
- $h_i = \text{molar specific enthalpy of constituent 'i'}$
- $k = \text{thermal conductivity of the mixture}$
- $C_{p_s} = \sum \alpha_i c_{p_i} = \text{specific heat of heavy particles}$
  - where the summation includes only the heavy particles.
- $c_{p_i} = \text{molar specific heat at constant pressure for constituent 'i'}$
- $C_{p_e} = \text{specific heat of electrons}$
- $D = \text{effective mixture diffusion coefficient (see Section 2.4.7)}$
- $\alpha_i = \text{concentration of plasma constituent 'i'}$
- $\alpha_e = \text{concentration of the electrons}$
- $T_e = \text{electron temperature}$.

Equation (2.9) is one of the energy equations required to represent the two-temperature system modeled in the nonequilibrium CAPS code.
An equation representing the energy in the electron gas is the other equation chosen to represent the energy in the two-temperature system. In this equation, the electrical Ohmic heating is balanced by electron conduction, convection, diffusion, and energy transport to the heavy particles through collisions [54]. The form of the equation is taken from Park [60].

\[
\nabla \cdot \rho \nabla \alpha_h e - \nabla \cdot [k_e \nabla T_e + h_e D \nabla \alpha_e] - \nabla \cdot \nabla p_e = S \quad (2.10)
\]

where \( S = q_{ce} + q_{ch} + q_i - q_r \). The last term on the left hand side of equation (2.10) describes the work done by the electron-pressure gradients. This term is determined using the assumption that the velocities of the heavy species and electrons are the same in the flow. The partial pressure of the electrons is given by [54]

\[
p_e = \frac{p_{T_e} x_e}{T_h + (T_e - T_h) x_e} \quad (2.11)
\]

where \( x_e \) is the electron mole fraction.

"The term \( q_{ce} \) represents the transfer of energy between the heavy gas and the electron gas resulting from collisions of electrons with heavy species," [54]

\[
q_{ce} = \sum_i^{\text{h.p.}} 2n_e \frac{m_e}{m_i} \nu_i \frac{3}{2} k(T - T_e) \quad (2.12)
\]

where \( \nu_i \) is the collision frequency and the summation is over the species in the heavy gas. "The collision frequency is evaluated from the temperature dependent collision cross-sections for electron-heavy collisions evaluated at the electron temperature using the transport property [routines] described in Section 2.4." [54]

Energy transport to the electron gas due to electron participation in chemical reactions is represented by the term, \( q_{ch} \), in equation (2.10). The energy released by a
three body recombination reaction with the electron acting as the third body is assumed to be absorbed into the electron gas, raising the electron temperature. Ionization and dissociation due to electron collision is assumed to remove the dissociation or ionization energy from the electron gas, lowering the electron temperature [54].

The electrical energy input to the system, \( q_i \), is the same Ohmic heating \( (J^2/\sigma) \) used in the equilibrium simulation. The optically thin radiation is represented by \( q_r \) and is the same for both the equilibrium and nonequilibrium simulations. The thermodynamic and nonequilibrium transport properties are discussed in Section 2.4.

### 2.2 Boundary Conditions

The radial gradients of \( u, H, h_e \) (in the nonequilibrium case), and \( p \) are set equal to zero on the symmetry axis (centerline). A no-slip condition is forced by specifying that the axial velocity is zero at the wall. The wall has a specified temperature and is assumed to be catalytic for electron-ion recombination and hydrogen atom recombination. This results in an equilibrium condition at the wall with the gas enthalpy specified by the pressure and the wall temperature. This equilibrium condition at the wall is used in the nonequilibrium plasma as well as the equilibrium plasma [54].

### 2.3 Species

Because the equilibrium CAPS code assumes LTE and chemical equilibrium, species concentrations are a function of pressure and temperature. These concentrations are defined by the Saha equation [61], a form of the law of mass action, which assumes all chemical reactions have equilibrated. The Saha equation cannot be
used to obtain nonequilibrium species concentrations since the time scales are too short for chemical reactions to be complete. For this case, finite rate chemical kinetics must be included in the CAPS code model.

For the nonequilibrium CAPS code, the system of governing equations (Section 2.1) are expanded to include three species equations to allow the calculation of systems where ionization of \( H \) and the dissociation of \( H_2 \) are not in equilibrium \([54]\). The hydrogen system is modeled as a four component system: molecular hydrogen, \( H_2 \); atomic hydrogen, \( H \); hydrogen ions, \( H^+ \); and electrons, \( e \). Because the system is electrically neutral, the electrons and hydrogen ions can be represented by the same species conservation equation (this allows the four species system to be modeled by three species concentration equations). The species conservation equation used in the CAPS code is \([54]\]

\[
\nabla \cdot \rho \bar{v} \alpha = \nabla \cdot \rho D \nabla \alpha + S_{\alpha} \tag{2.13}
\]

where \( \alpha \) is the concentration of the species under consideration, \( D \) is the effective mixture diffusion coefficient (discussed in Section 2.4.7), and \( S_{\alpha} \) is the production of the species by chemical reaction. Since the species are assumed to vary only radially, and the radial velocity is zero, the term on the left side of equation (2.13) is zero. Because of constraints in the SIMPLE algorithm, the source term \( S_{\alpha} \), must be evaluated before the species equations can be solved. If each grid cell is assumed to be a well-stirred reactor, the time available for chemical reactions to occur would be the characteristic time for a well-stirred reactor. The characteristic time for a well-stirred reactor is calculated from the mass in the computation cell of interest divided by the mass flux into the cell \([54]\). The nonlinear nature of the chemical rate equations,
however, requires that the species production be evaluated using a much smaller time step—the chemical time step—which is a fraction of the characteristic time for a well-stirred reactor. The species conservation equations—equation (2.13)—are then solved over this time step using a linearized set of equations for the four hydrogen species [62]. The source term ($S_{\alpha}$) for each cell is equal to the change in species concentration divided by the chemical time step.

The species production needed in the above calculation is calculated from chemical kinetic reaction rate coefficients. The forward reaction rate coefficients are calculated from the Arrhenius equation [63]

$$k_f = AT^{-n} \exp(E/RT) \quad (2.14)$$

where

- $A = \text{Arrhenius constant}$
- $E = \text{activation energy}$
- $R = \text{universal gas constant}$
- $T = \text{temperature}$.

The Arrhenius constant, the activation energy, and the power of the temperature, $n$, are user input to the computer program. The backward kinetic reaction rate coefficients, $k_b$, are calculated from $k_f$ and the equilibrium constant, $K_p$ [63].

$$k_b = -\frac{k_f}{K_p} \quad (2.15)$$

The calculated reaction rates can vary greatly for a chemical reaction depending upon the kinetic rate constants used in equation (2.14). The species concentrations obtained from the computer simulations are extremely sensitive to the calculated rate constants.
Furthermore, a significant amount of the energy is transported between the electrons and the heavy species when an electron acts as the third body in a reactive collision [64]. As a result, the recombination reaction rates can influence the electron to heavy gas temperature ratio, as well as the gas composition. The reaction rates for the hydrogen system used in the computer simulations in this work are presented in Chapter 4, along with simulation results.

2.4 Transport Properties

The transport properties for both the equilibrium and nonequilibrium versions of the UTSI cascade arc computer code are calculated using a computer code written by Cho [11] based on the procedures developed by DeVoto [65]. The transport property models used in this reference are based on the Chapman-Enskog method [66, 67]. The models in Cho's code start with experimental or calculated energy dependent collision cross-sections, calculate the collision integrals based on one of several interaction models and use combinations of the collision integrals to determine the transport properties. Electrical conductivity and electron thermal conductivity depend on collisions between electrons and heavy species in the mixture, while viscosity and heavy gas thermal conductivity depend primarily on collisions between the heavy species [64].

The Cho model makes the following assumptions when used with a two-temperature nonequilibrium plasma model. The fundamental cross-section data describes the interaction of one atom or molecule with another, and depends only upon collision energy and the identity of the colliding pair. The nonequilibrium plasma is described by a two-temperature model where a Maxwellian distribution at a unique electron temperature describes the kinetic energy of the electrons. The electron
temperature is used to determine the collision energy for all collisions involving electrons, since the relative velocity of a collision involving an electron is close to the velocity of the electron. The heavy gas temperature is used to determine the collision energy for all other collisions [64].

2.4.1 Collision Integrals

The transport property equations in Sections 2.4.1 through 2.4.6, detailing the calculations of the transport properties, are taken largely from Cho [11]. The collision integral between species i and j is [67]

\[
\Omega_{ij}^{(t,s)} = \frac{1}{2} \left( \frac{kT}{2\pi\mu_{ij}} \right)^{\frac{1}{2}} \int_{0}^{\infty} \exp(-x)x^{s+1}Q^t(\varepsilon)dx. \tag{2.16}
\]

where

\[
x = \varepsilon/kT
\]

\[
\varepsilon = \text{a relative translational energy between particles i and j}
\]

\[
\mu_{ij} = \text{the reduced mass}
\]

\[
Q^t(\varepsilon) = \text{the momentum transfer cross section.}
\]

The integer values of indices t and s vary depending on which transport property is being calculated (see Sections 2.4.2 through 2.4.6). The collision integral can be expressed in terms of both the temperature and the intermolecular or the interatomic potential, depending on the type of potential function associated with the colliding particles. For a given potential function, the angle of deflection of the colliding particles must be calculated. If the colliding particles are assumed to be rigid spheres,
the angle of deflection can be represented by an analytical expression, making the collision integral fairly easy to determine. The collision integral for colliding rigid spheres is given by [67]

\[
\Omega_{ij}^{(t,s)} = \frac{1}{2} \left( \frac{kT}{2\pi\mu_{ij}} \right)^2 (s + 1)^{l} \left[ \frac{2l + 1 - (-1)^{l}}{2(1+l)} \right] \pi d^2 \tag{2.17}
\]

where \( d \) is the diameter of the rigid sphere. However, any realistic collision potential functions must be calculated using numerical methods [67]. By dividing the collision integral in equation (2.16) by the collision integral for rigid spheres--equation (2.17)--a nondimensional form of the collision integral is obtained. This nondimensional integral, \( \Omega_{ij}^{(t,s)} \), shows "the deviation of any particular molecular model from the idealized rigid-sphere model" and allows easy incorporation of the potential function parameters [67].

\[
\Omega_{ij}^{(t,s)} = \frac{2(t+1)}{d^2 \pi (s+1)!} \int_{0}^{\infty} \exp(-x)x^{s+1}Q'(\epsilon)dx. \tag{2.18}
\]

A convenient form of the collision integral is defined as [11]

\[
\overline{\Omega}_{ij}^{(t,s)} = d^2 \Omega_{ij}^{(t,s)} \tag{2.19}
\]

Collision integrals for various potential functions have been tabulated in the literature and are used in the transport property routines. The potential functions available are:
exponential repulsive, Lenard-Jones, polarization, Morse, static exchange, and shielded Coulomb [67, 68-73]. The Cho [11] transport property routines used in the CAPS code use interatomic and intermolecular potentials reviewed by Aubreton [74].

2.4.2 Viscosity

The first approximation of the Chapman-Enskog approximation for viscosity is [67]

\[
\mu = -\frac{H_{22} x_2 + \ldots + H_{2N} x_2}{H_{N2} x_2 + \ldots + H_{NN} x_N}
\]

(2.20)

where \( H_{ij} \) are

\[
H_{ii} = \frac{x_i^2}{\eta_{ii}} + \sum_{k=2, k \neq i}^{N} \frac{2x_i x_k}{nD_{ik}(m_i + m_k)} \left( 1 + \frac{3m_k}{5m_i} A_{ik}^* \right)
\]

\[
H_{ij} = -\frac{2x_i x_j}{nD_{ij}(m_i + m_j)} \left( 1 - \frac{3}{5} A_{ij}^* \right)
\]
\[ \eta_{ii} = \frac{5}{16\sqrt{\pi}} \frac{m_i k T_i}{\Omega_i^{(2,2)}} \]

\[ A_{ij}^* = \frac{\Omega_{ij}^{(2,2)}}{\Omega_{ij}^{(1,1)}} \]

\( x_i \) and \( x_j \) are the mole fractions of species \( i \) and \( j \), and \( m_i \) and \( m_j \) are the masses of these species. \( n \) is the total number density, and \( D_{ij} \) are the binary diffusion coefficients presented in Section 2.4.6. This formulation is independent of electron number density.

### 2.4.3 Electron Thermal Conductivity

Electron-electron collisions and electron-heavy particle collisions contribute to electron thermal conductivity. The third approximation to the Chapman-Enskog approximation is [75]

\[ k(e) = \frac{75}{8} n_1^2 \left( \frac{2 \pi k T_e}{m_1} \right)^2 \frac{1}{q^{(1,1)} q^{(2,2)} - q^{(1,2)} q^{(1,2)}} q^{(2,2)} \]

(2.21)

where

\[ q^{(1,1)} = 8 \pi \sqrt{2} n_1^2 \Omega_{11}^{(2,2)} + 8 \pi n_1 \sum_{i=2}^{N} n_i \left( \frac{25}{4} \Omega_{ii}^{(1,1)} - 15 \Omega_{ii}^{(1,2)} + 12 \Omega_{ii}^{(1,3)} \right) \]
where \( m_i \) and \( n_i \) are the electron mass and electron number density, respectively. \( n_i \)
represents the number densities of the heavy species.

### 2.4.4 Thermal Conductivity of Heavy Particles

The thermal conductivity of the heavy particles is [67, 72]

\[
k_{(g)} = \begin{pmatrix}
L_{22} & \cdots & L_{2N} & x_2 \\
\vdots & \ddots & \vdots & \vdots \\
L_{N2} & \cdots & L_{NN} & x_N \\
x_2 & \cdots & x_N & 0
\end{pmatrix}
\]  

(2.22)
where

\[ L_{ii} = \frac{-4x_i^2}{\lambda_{ii}} - \frac{16x_i x_k}{25n_k D_{ik}(m_i + m_k)^2} \left( \frac{15}{2} m_i^2 + \frac{25}{4} m_k^2 - 3m_k^2 B_{ik}^* + 4m_i m_k A_{ik}^* \right) \]

\[ L_{ij} = \frac{16x_i x_j m_i m_j}{25n_k D_{ij}(m_i + m_j)^2} \left( \frac{55}{4} - 3B_{ij}^* - 4A_{ik}^* \right) \]

\[ \lambda_{ii} = \frac{75}{64\sqrt{\pi}} \left( \frac{k^2}{\Omega_{ij}^{(2,2)}} \right)^{\frac{1}{2}} \frac{T_i}{m_i} \]

\[ B_{ij}^* = \frac{5\Omega_{ij}^{(1,2)} - 4\Omega_{ij}^{(1,3)}}{\Omega_{ij}^{(1,1)}} \]

### 2.4.5 Electrical Conductivity

According to DeVoto [75, 76], the third approximation for electrical conductivity is
\[ \sigma = \frac{3}{2} e^{2} n_{1}^{2} \sqrt{\frac{2\pi}{m_{1} k T_{e}}} \frac{q^{(1,1)} q^{(2,2)} - q^{(1,2)} q^{(1,2)}}{D_{q}} \] (2.23)

where

\[ D_{q} = q^{(0,0)} \left[ q^{(1,1)} q^{(2,2)} - q^{(1,2)} q^{(1,2)} \right] + q^{(0,1)} \left[ q^{(1,2)} q^{(0,2)} - q^{(0,1)} q^{(2,2)} \right] + q^{(0,2)} \left[ q^{(0,1)} q^{(1,2)} - q^{(0,2)} q^{(1,1)} \right] \]

\[ q^{(0,0)} = 8\pi n_{1} \sum_{i=2}^{N} n_{i} \Omega^{(1,1)}_{ii} \]

\[ q^{(0,1)} = 8\pi n_{1} \sum_{i=2}^{N} n_{i} \left( \frac{5}{2} \Omega^{(1,1)}_{ii} - 3\Omega^{(1,2)}_{ii} \right) \]

\[ q^{(0,2)} = 8\pi n_{1} \sum_{i=2}^{N} n_{i} \left( \frac{35}{8} \Omega^{(1,1)}_{ii} - \frac{21}{2} \Omega^{(1,2)}_{ii} + 6\Omega^{(1,3)}_{ii} \right) \]

2.4.6 Binary Diffusion Coefficient

Hirschfelder et al. [67] give the binary diffusion between species i and j to be

\[ D_{ij} = \frac{3}{16} \sqrt{\frac{2kT}{\mu_{ij}}} \frac{1}{n\Omega^{(1,1)}_{ij}}. \] (2.24)

where \( n \) is the total number density in the plasma.
2.4.7 Ambipolar Diffusion

In a plasma, the electrons tend to diffuse at a faster rate than ions because the electrons have a much smaller mass than the ions. This faster electron diffusion results in a charge separation between the electrons and ions. The resulting electrostatic field retards the diffusion of the electrons and boosts the diffusion of the ions. The internal electrostatic field ultimately forces the electrons and ions to diffuse at the same rate. This diffusion process is known as ambipolar diffusion [77] and only effects the diffusion rate of charged particles. The ambipolar diffusion process is assumed in the UTSI CAPS code, where applicable. For monatomic plasmas in LTE, ambipolar diffusion is [76]

\[
D_{\text{ambi}} = 2D_{\text{ia}} \left[ 1 - \frac{m_e D_{\text{ie}}}{m_i D_{\text{ia}}} \left( 1 - \frac{D_{\text{ea}}}{D_{\text{ei}}} \right) \right].
\]  

(2.25)

where

- \(D_{\text{ia}}\) = binary diffusion coefficient of ions in atoms
- \(D_{\text{ie}}\) = binary diffusion coefficient of ions in electrons
- \(D_{\text{ea}}\) = binary diffusion coefficient of electrons in atoms
- \(m_e\) = electron mass
- \(m_i\) = ion mass.

For the conditions seen in the CAPS code simulations, the term in the brackets of equation (2.25) is approximately equal to one. Therefore, equation (2.25) becomes

\[
D_{\text{ambi}} \equiv 2D_{\text{ia}}.
\]  

(2.26)
Ambipolar diffusion is essentially two times faster than the diffusion of the ions in the atoms. For plasma gases not in LTE, the ambipolar diffusion is [77]

\[ D_{\text{ambi}} \equiv \left(1 + \frac{T_e}{T_g}\right)D_{\text{ia}}. \]  (2.27)

Species diffusion in the CAPS code utilizes the binary diffusion coefficients, and ambipolar diffusion coefficients are used where positively charged particles (\(H^+\)) and negatively charged particles (\(e\)) diffuse. In the plasma flows seen in a cascade arc, it is assumed that there are very few locations where \(H_2\) and the ion/electron pair coexist. Therefore, a single effective diffusion coefficient is used in the CAPS code for all species rather than the correct, but much more complicated, multicomponent diffusion coefficients [54]. Multicomponent diffusion coefficients are not used in the CAPS code because they result in species conservation equations composed entirely of nonlinear cross-species terms. This nonlinear interdependence creates a very difficult computational problem that can, in theory, be solved. However, the SIMPLE algorithm used in the CAPS code cannot solve conservation equations in this form. To formulate the species conservation equations in a manner that can be solved by SIMPLE, Rhodes [54] created a heuristic mixture rule to provide an effective diffusion coefficient that allows a smooth transition across regions where all four components \((H_2, H, H^+, e)\) coexist.

\[
D = \frac{\left[ \alpha_{H_2} \alpha_H D_{H_2H} + \left(\alpha_{H_2} \alpha_{H^+} + \alpha_{H_2} \alpha_e\right)D_{H_2H^+} \right]}{\left(\alpha_{H_2} \alpha_H + \alpha_{H_2} \alpha_{H^+} + \alpha_{H_2} \alpha_e + \alpha_H \alpha_{H^+} + \alpha_H \alpha_e\right)}
+ \left(\alpha_H \alpha_{H^+} + \alpha_H \alpha_e\right)D_{HH^+}.
\]  (2.28)
The diffusion coefficients for the $H^+/H_2$ pair and the $H^+/H$ pair in equation (2.28) are ambipolar diffusion coefficients calculated using equation (2.27). Ambipolar diffusion causes the electrons to diffuse into $H_2$ and $H$ at the same rate as the ions. Therefore, separate binary diffusion coefficients involving electrons are not required—the CAPS code models an electrically neutral plasma, $\alpha_e = \alpha_{H^+}$. Equation (2.28) gives the correct answer for any two-component mixture and provides a smooth transition where the mixture has three components [54]. The effective diffusion coefficient given by equation (2.28) is used in the nonequilibrium energy equations—equations (2.9) and (2.10)—and the conservation of species equation—equation (2.13).

### 2.4.8 Radiation Transport

Radiation transport is calculated using the methods described by Griem [61] which include both line and continuum emission. Energy transport through radiation is modeled as having an optically thin part and an optically thick part. The optically thin radiation is not absorbed back into the plasma gas and is assumed to result in a direct energy loss from the plasma to the constrictor wall of the cascade arc. The optically thick component is absorbed back into the plasma gas and is modeled as a thermal conductivity using the Rosseland approximation [78]. The Rosseland approximation models optically thick radiation transport with the equation

$$q_z = -\frac{16}{3a_R} \sigma T^3 \frac{\partial T}{\partial z}$$  \hspace{1cm} (2.29)$$

where $a_R$ is the **Rosseland mean absorption coefficient** given by

$$\frac{1}{a_R} = \int_0^\infty \frac{1}{a_\lambda(\lambda)} \frac{\partial e_{\lambda b}}{\partial \lambda} d\lambda.$$
where

$$\frac{\partial a_\lambda}{\partial e_b} = \frac{\pi C_1 C_2 \sigma^{1/4}}{2} \frac{e_b^{5/4}}{e_b} \frac{\exp\left[(C_2/\lambda)(\sigma/e_b)^{1/4}\right]}{\left[\exp\left[(C_2/\lambda)(\sigma/e_b)^{1/4}\right]-1\right]^{2}}.$$ 

and

- $a_\lambda$ = spectral absorption coefficient,
- $\lambda$ = wavelength,
- $\sigma = $ Stefan-Boltzmann constant = 5.57051E-8 W/(m²-K),
- $C_1 = 0.59552197E+8$ W·µm⁴/(m²-sr),
- $C_2 = 14,387.69$ µm·K,
- $e_b = \sigma T^4$.

Using (2.29), the Rosseland thermal conductivity, $k_R$, is

$$k_R = \frac{16}{3a_R} \sigma T^3$$ (2.30)

This Rosseland thermal conductivity is fitted as a function of mixture enthalpy, electron concentration, and pressure for a hydrogen plasma in equilibrium. The resulting equation is used in the nonequilibrium code [54]. Any error associated with this assumption is assumed to be small because optically thick radiation is very small when compared to the other energy transport mechanisms in hydrogen plasmas at pressures and temperatures realized in the UTSI cascade arc. The Rosseland thermal conductivity—equation (2.30)—is added to the internal thermal conductivity of the heavy species to form an effective thermal conductivity for use in the CAPS code simulations when thermal equilibrium is assumed. Otherwise, the Rosseland
component is added to the electron thermal conductivity to form an effective electron thermal conductivity.

2.5 Thermodynamic Properties

The thermodynamic properties can be determined if both the partition function and the composition of the plasma are known. In general, the partition function of a plasma is the product of the internal partition function, the translational partition function, the rotational partition function, and the vibrational partition function.

$$Q_{\text{total}} = Q_{\text{int}} \cdot Q_{\text{trans}} \cdot Q_{\text{vib}} \cdot Q_{\text{rot}}$$

(2.31)

The internal partition function is given by [9]

$$Q_{\text{int}} = \sum_{i=0}^{N} g_i \exp \left( \frac{-\varepsilon_i}{kT} \right),$$

(2.32)

where

$$\varepsilon_i = \text{energy associated with the } i^{\text{th}} \text{ major quantum level},$$

$$g_i = \text{statistical weight or degeneracy associated with the } i^{\text{th}} \text{ energy level},$$

$$k = \text{the Boltzmann constant},$$

$$T = \text{excitation temperature of atom or molecule},$$

$$N = \text{the last major quantum level before a bound electron can escape the atom or molecule}.$$}

The translational partition function is given by [9]

$$Q_{\text{trans}} = V \left( \frac{2\pi mkT}{\hbar^2} \right)^\frac{3}{2}$$

(2.33)
where

\[ V = \text{the volume occupied by the plasma}, \]
\[ m = \text{the mass of the atom or molecule}, \]
\[ h = \text{Plank's constant}. \]

The vibrational partition function is [13]

\[ Q_{\text{vib}} = 1 + \sum_{v=1}^{\infty} \exp \left( \frac{-G_0(v)hc}{kT} \right) \]  \hspace{1cm} (2.34)

where

\[ G_0 = \text{energy associated with vibration state } v. \]
\[ c = \text{the speed of light}. \]

The rotational partition function is [13]

\[ Q_{\text{rot}} = \int (2J + 1) \exp \left( \frac{-hcBJ(J + 1)}{kT} \right) dJ = \frac{kT}{hcB} \]  \hspace{1cm} (2.35)

where

\[ J = \text{total angular momentum quantum number}, \]
\[ B = \text{the rotational constant for the molecule [13].} \]

The vibrational and rotational partition functions are both zero for atoms. Therefore, only diatomic hydrogen will have nonzero values for these quantities.

After the total partition function has been evaluated, the thermodynamic properties can be determined. The Helmholtz potential, \( F \), and the Gibbs potential, \( G \), can be calculated using [79]

\[ F = -kT \ln Q_{\text{total}} \]  \hspace{1cm} (2.36)

and

\[ \text{42} \]
\[ G = F + PV \]  
(2.37)

where \( P \) is pressure.

The entropy, \( S \), is calculated using the Gibbs potential [79].

\[ S = -\left( \frac{\partial G}{\partial T} \right)_P \]  
(2.38)

The enthalpy, \( H \), is calculated using [79]

\[ H = G + TS. \]  
(2.39)

The specific heat at constant pressure is obtained using [79]

\[ C_p = T \left( \frac{\partial S}{\partial T} \right)_P. \]  
(2.40)

By substituting equations (2.31), (2.36) through (2.38) into equations (2.39) and (2.40), the constant pressure specific heat and enthalpy can be shown to be [80]

\[ C_p = R \left[ \frac{T^2}{Q_{tot}} \frac{d^2Q}{dT^2} - \left( \frac{T}{Q_{tot}} \frac{dQ}{dT} \right)^2 + \frac{2T}{Q} \frac{dQ}{dT} + \frac{5}{2} \right] \]  
(2.41)

and

\[ H = H_0 + RT \left( \frac{T}{Q} \frac{dQ}{dT} + \frac{5}{2} \right) \]  
(2.42)

where \( R \) is the universal gas constant and \( H_0 \) is the chemical energy at 0 K for the standard state. The equilibrium and nonequilibrium CAPS codes both calculate the enthalpy and the specific heat at constant pressure using tabulated coefficients.
determined from fifth order polynomial curve fits to data calculated \textit{a priori} using equations (2.41) and (2.42) \cite{80}. Mixture enthalpy and mixture $C_p$ are covered in Sections 2.1.2 and 2.1.3.
CHAPTER 3

EXPERIMENTAL SETUP AND PROCEDURE

This chapter contains a detailed description of the UTSI Cascade Arc Facility. The design, fabrication, and construction of the facility are presented along with details of problems encountered while bringing the facility on-line. The chapter closes with facility operation guidelines and experimental procedure.

3.1 Experimental Setup

The UTSI cascade arc is comprised of individually water cooled copper plates separated by electrical insulators (Figure 3.1). These plates are 1/8" thick and form a 4 mm diameter arc channel that is approximately 40 mm long. The insulators are ceramic paper or mica 0.010" thick. A modified plate with windows allows optical access. This section is located in the center of the cascade arc to minimize end effects. The cathode is a 0.250" diameter thoriated tungsten rod with a 60 degree cone on the end. The anode is 0.360" diameter thoriated tungsten rod with a blunt end. Both electrodes are cooled by a water jet impinging on their back surface. The arc is driven by a 50 A, 600 V power supply. A cascaded centrifugal pump delivers 11 gal/min of water at 200 psi to cool the copper plates and electrodes. The cascade arc is positioned vertically to eliminate arc asymmetries caused by buoyancy.
3.1.1 Design and Fabrication of UTSI Cascade Arc Apparatus

This section will give details of the major components of the UTSI Cascade Arc apparatus. A picture of the assembled apparatus is shown in Figure 3.2. A discussion of the design and fabrication of each component follows. Detailed drawings of each component designed at UTSI can be found in Appendix A.

3.1.1.1 Constrictor Plates

The copper constrictor plates form the arc constrictor channel through which the arc passes. Each plate is made of oxygen free, high conductivity (OFHC) copper and is square with 1.25" sides and has a thickness of 1/8". In addition to the central 4 mm diameter constrictor hole, the plate has a hole in each corner to accommodate a 1/4" diameter, G10 bolt that will hold the assembled cascade together. A circular groove for an o-ring surrounds the constrictor hole. Water cooling is supplied through a channel cut into the constrictor plate.

Figure 3.1 Diagram showing the components of the UTSI cascade arc apparatus.
Figure 3.2 Picture of the UTSI Cascade Arc assembly.
Figure 3.3 is a schematic of the cooling water path through a constrictor plate. Arrows indicate the direction of flow. The cooling water enters through a 1/16" diameter inlet channel and travels radially inward to a circular channel with a radius between the radii of the central constrictor hole and the o-ring groove. This circular channel has a rectangular cross-section 0.040" wide and 0.080" deep. It forms an almost complete circle around the constrictor hole and empties into a 1/16" diameter water outlet channel that exits radially from the constrictor plate. The inner, water cooling channel is cut into the face of the constrictor plate using a milling machine, and the water inlet and outlet channels are drilled into the plate through one edge. The central channel is closed using an OFHC washer cap that is silver brazed into place. Stainless steel nipples were designed to fit into the inlet and outlet channels. Once silver brazed into place, these nipples allow the constrictor plate to be clamped onto 1/8" diameter nylon tubing using a small hose clamps. A picture of the plate after being fitted with the washer cap and nipples appears in Figure 3.4. The constrictor plate, the washer cap, and the fittings were all designed and fabricated in-house at UTSI.

To ensure proper operation of the cascade arc, the water cooling channels must be designed to adequately remove all of the electrical power load deposited into the plasma. In the design process, the power load was calculated using

\[ P_{\text{load}} = I^2EL \]  

(3.1)

where

- \( I \) = current [A]
- \( E \) = the electric field [Volts/cm]
- \( L \) = the thickness of the constrictor plate [cm].

The load power was assumed to be a hydrogen arc at 50 A and 1 atmosphere—the most intense arc anticipated for the UTSI cascade arc. The electric field was taken to be 90 V/cm [22] for a 50 A hydrogen arc at 1 atm. The resulting power load is 1750 Watts for each disk.
Figure 3.3 Schematic of the cooling water path in a constrictor plate.
Figure 3.4 Picture of an assembled constrictor plate.
Therefore, the cooling water for each disk must be able to remove this power for steady state operation of the cascade arc.

The water cooling channels were designed to flow 0.82 gal of water per minute at a 200 psi inlet pressure. The resulting flow has a bulk speed of about 25 m/s. The pressure in the channel reduces as the channel exit is approached. To determine the size and capacity needed for the cooling water pump, the pressure drop through the water cooling channel was needed. The pressure drop was calculated using [81]

\[ \Delta P = \frac{f \rho u^2}{2} \left( \frac{L_c}{D_h} \right) \]  

(3.2)

where

- \( f \) = the turbulent friction factor taken from the Moody diagram
- \( L_c \) = the length of the cooling water channel
- \( \rho \) = the fluid density
- \( u \) = the speed of the fluid
- \( D_h \) = the hydraulic diameter = \( \frac{4A_c}{P} \)
- \( A_c \) = the channel cross-section
- \( P \) = the perimeter of the channel cross-section.

The velocity and associated pressure drops vary between plates because the silver brazing results in slight changes in the cooling channel cross-sections.

The convective heat transfer coefficient was very important in designing the water cooling channel. Convective heat transfer coefficients were calculated from two different Nusselt number correlations that are appropriate for the water flow conditions in the cooling
channel. The correlation that resulted in the lowest heat transfer was used as a conservative value in the design process. One of the correlations was taken from Incropera et. al. [81]

\[
\text{Nu}_D = \frac{(f/8)(Re_D - 1000)Pr}{1 + 12.7(f/8)^{1/2}[Pr^{2/3} - 1]}
\]

(3.3)

for fully developed turbulent flow for which

\[
0.5 < Pr < 2000
\]

\[
2300 < Re_D < 5.0E+6
\]

where

\[
Pr = \text{the Prandtl number}
\]

\[
Re_D = \frac{\rho u_D h}{\mu} = \text{the Reynolds number}
\]

\[
\mu = \text{the dynamic viscosity.}
\]

The other Nusselt number correlation used in the design process is the Petukhov equation [82]

\[
\text{Nu} = \frac{Re_D Pr \left(\frac{f}{8}\right) \left(\frac{\mu_b}{\mu_w}\right)^n}{\chi}
\]

(3.4)

where

\[
\chi = 1.07 + 12.7(Pr^{2/3} - 1)\left(\frac{f}{8}\right)^{1/2}
\]

and

\[
n = \begin{cases} 
0.11 & \text{heating (}T_w > T_b\text{)} \\
0.25 & \text{cooling (}T_w < T_b\text{)} \\
0 & \text{gases}
\end{cases}
\]
for fully developed turbulent flow in the range

\[ 1.0 \times 10^4 < \text{Re}_D < 5.0 \times 10^6 \]

\[ 2 < \text{Pr} < 140 \quad \text{with 5 to 6 percent error} \]
\[ 0.5 < \text{Pr} < 2000 \quad \text{with 10 percent error} \]

\[ 0.08 < \frac{\mu_w}{\mu_b} < 40. \]

All physical properties are evaluated at the bulk temperature, except for \( \mu_w \).

The convective heat transfer coefficient, \( h \), is calculated from the above Nusselt number, \( \text{Nu} \), using

\[ h = \frac{k\text{Nu}}{D_h}. \quad (3.5) \]

where \( k \) is the Fourier coefficient of heat conduction of the fluid.

The temperature rise from the inner wall of the cooling channel to the cooling water was calculated using

\[ T_{\text{wall}} - T_{\text{water}} = \frac{\dot{q}}{hA}. \quad (3.6) \]

where

\( \dot{q} = \) heat transfer from the cascade wall to the cooling water,
\( A = \) the surface area of the inner surface of the cooling channel.

In the design process the water temperature used in equation (3.6) was taken to be the water temperature at the exit of the water cooling channel. This wall temperature was calculated using

\[ T_{\text{water}} = T_{\text{water in}} + \frac{\text{P}_{\text{load}}}{\dot{m} C_p} \quad (3.7) \]
where \( \dot{m} \) and \( C_P \) are the mass flow rate and specific heat at constant pressure for the water.

The heat transfer in equation (3.6) was taken to be the heat addition to the water flow associated with the onset of nucleate boiling. In general, if the temperature of the water reaches the saturation temperature, \( T_s \), at local water pressure, the water will start changing to gas. In the case where water is cooling a hot wall, nucleate boiling will occur if the wall temperature exceeds a temperature, \( \Delta T_{\text{sat}} \), above the saturation temperature. Whalley [83] gives the following empirical correlation for this shift in saturation temperature.

\[
\Delta T_{\text{sat}} = T_{\text{sat}} + \frac{8\sigma T_{\text{sat}} \phi}{\lambda \rho_g k_1}
\]  

(3.8)

where

\( \sigma \) = surface tension

\( \lambda \) = latent heat of vaporization

\( \phi \) = heat flux = \( \frac{\dot{q}}{A} \)

\( \rho_g \) = gas density

\( k_1 \) = thermal conductivity of the liquid.

If the wall temperature exceeds the shifted saturation temperature \( (T_{\text{sat}} + \Delta T_{\text{sat}}) \), nucleate boiling will occur.

Beyond nucleate boiling, film boiling may occur causing cavitation in the water cooling channel. This would lead to gaseous pockets next to the inner wall of the channel; heat transfer to the water would be greatly reduced and lead to the ultimate destruction of the
constrictor plate. To ensure that film boiling will not occur, the following correlation was utilized in the design process [83]

\[ \varphi_{\text{crit}} = A \lambda G^{1/2}(1 - X) \] (3.9)

where

\( \varphi_{\text{crit}} \) = the critical heat flux associated with the onset of nucleate boiling

\( X \) = the fraction of mass flow that is gas = 0

\( G \) = the mass flux

\( A = 0.25 \text{ kg}^{-0.5} \text{m}^{-0.5} \) for water.

Film boiling will occur if the critical heat flux is exceeded. The critical heat flux, obtained from equation (3.9), was used as an additional check on the water cooling channel design. However, using the onset of nucleate boiling for an upper limit on the heat transfer should preclude the possibility of cavitation and the ultimate destruction of the plate. The area in equations (3.6) and (3.8) was chosen to be only the inner wall of the channel instead of the entire channel surface area. This adds a small factor of safety to the channel design.

For a final design check, the temperature of the constrictor wall was calculated from the steady state energy balance given in equation (3.10) --rearranged in equation (3.11)--to ensure that the constrictor wall temperature would remain well below the melting point of OFHC copper.

\[ \frac{d}{dr} \left( k_{\text{Cu}} A \frac{dT}{dr} \bigg|_{\text{wall}} \right) = 0 \] (3.10)

leads to
\[ T_{\text{constrictor}} = T_{\text{wall of water channel}} + \frac{P_{\text{load}}}{2\pi k_{\text{Cu}} L} \ln \frac{r_{\text{channel}}}{r_{\text{constrictor}}} \] (3.11)

where \( k_{\text{Cu}} \) is the Fourier coefficient of heat conduction for copper.

The design of the water cooling channel was optimized by varying the water inlet pressure, and the size and the shape of the cooling channels as parameters in equations (3.1) through (3.11). The final design was chosen as soon as the pressure and heat transfer requirements stated in this section were simultaneously satisfied. Much of the initial constrictor plate design analysis was performed using a spreadsheet. A sample plot of the calculated pressure drop—equation (3.2)—through the water cooling channel (1 mm by 2 mm cross-section) as a function of the water channel radius is shown in Figure 3.5. The speed of the cooling water is assumed to be 25 m/s. Figure 3.6 shows a sample plot of the calculated change in temperature at the inner wall of the cooling channel—equation (3.6)—as a function of the cooling channel radius. Dashed lines in the figure indicate the operating point of the final constrictor plate design. It is important to note, however, that this operating point is calculated for a hypothetical 50 A hydrogen arc at 1 atmosphere with a 90 V/cm axial electric field. This hypothetical arc results in heat loads more than a factor of two higher than those realized in the experiment. The overprediction of this heat load was anticipated, but was used in the analysis to introduce a factor of safety into the design. The chosen constrictor plate design prevents both nucleate boiling and film boiling while keeping water pressure losses in the water cooling channel at an acceptable level.
Figure 3.5 A design plot of the calculated pressure drop through the water cooling channel (1 mm by 2 mm cross-section) as a function of the water channel radius.
Figure 3.6 A design plot of the calculated change in temperature at the inner wall of the cooling channel (1 mm by 2 mm cross-section) as a function of the cooling channel radius.
3.1.1.2 Window Section

The window section constrictor plate is a version of the constrictor plate discussed in the last section that has been modified to accommodate four sapphire windows. These windows are 1 mm thick, 5 mm diameter disks that are situated on two mutually perpendicular axis that allow optical access to the plasma from two directions at the same time. This design feature was chosen to make laser induced fluorescence measurements possible. Pictures of the window section are shown in Figures 3.7 and 3.8. There is a notch in the two sides of the plate that do not have water cooling line nipples. A window is located in the recessed wall of each notch. This window location allows optical measurements to be made over a larger solid angle than is possible through the windows located between the nipples on the other two sides.

![Figure 3.7](image)

Figure 3.7 Picture of the window section showing the optical access between cooling line nipples.
The design process for the regular constrictor plates was repeated for the window section. The only difference is that the window section contains two water cooling channels, one on each side of the plate. The window section is constructed from two plates that are very similar to the regular constrictor plates. Once machined these plates are soft soldered together to form the window section. Finally, the sapphire windows are epoxied into sockets that are carefully machined into the window section at the end of each optical channel leading to the constrictor.

### 3.1.1.3 Insulator Gaskets and O-rings

An inner and an outer insulator gasket are placed between two adjacent constrictor plates to hold the o-ring in place and electrically isolate the plates. Both mica and ceramic paper gaskets are used in the cascade arc facility. The outer gasket is 0.010" thick mica and the inner gasket is 1/32" thick, binderless ceramic paper made of alumina and silica. A picture of the inner and outer gaskets along with an o-ring and a constrictor plate are shown in Figure 3.9. The inner gaskets are exposed to the plasma and must be replaced after extended use. One set of inner gaskets can last for several hours for an argon arc. Hydrogen arcs, however, are much more intense and cause failure of the inner insulator gasket in about 30
Figure 3.9 Picture showing gaskets, o-ring, and constrictor plate.

minutes. Replacement gaskets are readily available because they are cut out of sheet mica or ceramic paper in large quantities using the Center for Laser Applications carbon dioxide laser.

3.1.1.4 Electrodes

The electrodes are made out of 2 percent thoriated tungsten welding rods. The cathode is made by cutting a short length of a 1/4" diameter welding rod and grinding a 60 degree cone on one end. The flat end of the rod is silver soldered into the end of a 1/4" diameter stainless steel tube. Alignment of the cathode tip and the tubing is assured by a shoulder that is ground into the cathode tip at the location of the solder joint (see Appendix A for detailed drawings). A 1/8" thin-walled stainless steel tube is placed inside the larger tube and delivers cooling water to the back surface of the cathode tip (Figure 3.10). The cooling water is removed from the cathode via the annular region created by the two tubes.
Figure 3.10 Schematic of the cathode.
The anode and cathode designs are very similar. Both have water impinging on the back surface of the tungsten for cooling, and both have the same water delivery and return system. The tungsten anode, however, has a 0.380" diameter and a blunt end. A copper washer was designed to be soft soldered to the end of the inner, water delivery tube to force the water jet to flow over the entire back surface of the tungsten. The enclosure around the washer was machined from copper and soft soldered to the outer, water return tube. The thoriated tungsten anode is silver brazed to the copper enclosure (Figure 3.11). Like the cathode, alignment of the anode components is assured by shoulders that hold the components in place during soldering (see Appendix A for detailed drawings and construction details).

3.1.1.5 Electrode Housings

The cathode is held in place by the cathode housing (Figure 3.12). The cathode housing is made of OFHC copper and has a single water cooling channel identical to the one in the constrictor plates. The housing is electrically isolated from the constrictor plate adjacent to it using the insulator gaskets and o-ring discussed in Section 3.1.1.3. An annular, boron nitride shell is placed inside of the housing to thermally protect the G10 shell above it (G10 is a strong plastic that is easily machined). The G10 shell centers the cathode in the housing and accommodates o-rings to control the test gas environment. The cathode, G10 shell, and boron nitride shell are held in place by a brass, threaded, compression fitting with silicon ferrels which are electric insulators. The cascade arc test gas enters through three holes in the housing right above the water cooling channel. Multiple gas inlets allow the testing of a gas with different mixture ratios of as many as three kinds of gas stored in separate bottles. The G10 retaining bolts are screwed into four threaded holes in the bottom of the cathode housing.
Figure 3.11 Schematic of the anode.
Figure 3.12. Schematic of the cathode housing and the cathode.
The design of the anode housing is similar to that of the cathode housing (Figure 3.13). The anode is soft soldered directly to an anode cap that is electrically isolated from the anode housing by a G10 spacer. O-rings are utilized at these interfaces to isolate the test gas from atmospheric air. The test gas exits through two holes in the housing that are connected to a mechanical vacuum pump. The anode housing is cooled by a single water cooling channel identical to the one in the constrictor plate. The G10 retaining bolts pass completely through the anode housing, G10 spacer, and anode cap. Nuts are placed on the bolts and hold the cascade assembly together. For safety purposes, the anode is grounded, and the cathode floats at a negative potential.

Figure 3.13. Schematic of the anode housing and the anode.
3.1.1.6 **G10 Retaining Bolts**

The cascade arc apparatus is held together by four 1/4" diameter, G10 retaining bolts that screw into the cathode housing. Nuts are placed on the bolts after the anode cap and are tightened. The bolts are then attached to the translation table to support the cascade apparatus.

3.1.2 **Cascade Arc Apparatus Auxiliary Components**

The cascade arc apparatus is only one component in the UTSI Cascade Arc Facility. Other systems include the power, cooling, gas flow, and cascade translation systems. Each of these systems—necessary for cascade arc operation—are discussed in this section.

3.1.2.1 **Electrical Power System**

The heart of the power system is the EMHP 600-50 direct current power supply that delivers 0 to 50 A at 0 to 600 Volts. The output voltage and current are regulated to within 0.1 percent with variations in external load. Voltage and current are also stable to within 0.05 percent over eight hours [84]. The EMHP 600-50 can be operated in constant voltage or constant current mode. The constant current mode is used to drive the cascade arc.

Plasmas can have a negative current-voltage characteristic. Therefore, the voltage can decrease with increasing current. The power supply cannot stabilize the current to its set value in this situation, and the arc ceases. To allow the power supply to control the current in situations where the plasma has a negative current-voltage characteristic, the plasma must be put in series with a load that has a positive current-voltage characteristic large enough to make the overall system characteristic positive. A ballast resistor bank is put in series with the
cascade arc apparatus for this purpose. The resistor bank uses eight, 2 Ohm resistors arranged
to give 4 Ohms of resistance (see Figure 3.14). When the cascade arc is run at 50 A, 10 kW
of power are dissipated in the resistor bank. Without a cooling fan to remove this heat load,
the resistors could fail.

The 600 V available from the power supply is not enough to cause breakdown in the
test gas over the 40 mm length of the cascade arc constrictor. Therefore, a Tesla coil is used
to initiate the arc. Once the arc has started, enough free electrons are available to greatly
reduce the resistance between electrodes. This causes the plasma voltage to drop, and the
Tesla coil is no longer needed. The current is turned off at the power supply when shutting
down the arc plasma.

Figure 3.14. Arrangement of resistors in the ballast resistor bank.
3.1.2.2 Water Cooling System

A complex flow system is required to supply water to the cooling water channels in the cascade arc apparatus and carry away the heated water. In addition to the cooling channels in the cascade arc apparatus, the flow system is comprised of a pump, an inlet manifold, an outlet manifold, and a throttle valve to control the flow rate and pressure in the apparatus. Figure 3.15 is a diagram of the cooling water flow through the entire UTSI Cascade Arc Facility. Tap water is brought into the system from the laboratory cold water supply line and enters the pump. The pump increases the water pressure before it enters an inlet manifold. At this point, the flow is split into enough parallel lines for simultaneous

![Diagram of cooling water flow through the UTSI Cascade Arc Facility.](image)

Figure 3.15 Diagram of cooling water flow through the UTSI Cascade Arc Facility.
water delivery into each of the cascade arc cooling water channels. After exiting the cascade arc, the individual flow lines are brought back together in the outlet manifold. A throttle valve is located downstream of the outlet manifold to control cooling water pressure and flow rate. After passing the throttle valve, the heated cooling water is dumped (the rise in water temperature is less than two degrees Celsius).

The pump is a Grundfos multistage centrifugal pump, model CR4-160/14U, which delivers 20 gallons of water per minute at 200 psi to the inlet manifold pictured in Figure 3.16. The manifold is made of several 1/2" brass street tee unions brazed together. Swagelok reduction unions are brazed into the remaining openings in the street tees. 1/4" Nylon tubing is attached to these Swagelok compression fittings and delivers cooling water from the inlet to the cascade arc apparatus. Upon exiting the cascade apparatus, the heated water is brought back together in the outlet manifold shown in Figure 3.17. The outlet manifold is made in the same way as the inlet manifold, with the addition of a pressure gauge and a flow meter. Two type T thermocouples are placed on the inlet and outlet manifold lines that deliver and receive water from the same cooling water channel. This allows the rise in cooling water temperature for that channel to be measured. These thermocouples are visible in Figures 3.16 and 3.17. A thermocouple is also placed at the outlet manifold exit so that an overall increase in the cooling water temperature can be measured. This information, along with the volumetric flow rate, can be used to determine the amount of energy carried away by the cooling water. The manifold assembly hooked up to all of the nylon cooling water lines is shown in Figure 3.18.

It is desirable to keep the pressure high in the cascade arc cooling water channels to keep the water from boiling. Because the pressures in the outlet and inlet manifolds are, respectively, lower and higher than the pressure in the cascade arc apparatus, the pressure gauge is placed on the outlet manifold. As a result, a pressure gauge reading can establish a minimum pressure in the cascade arc. The throttle valve is opened to reduce the pressure and
Figure 3.16 The inlet manifold.

Figure 3.17 The outlet manifold.
increase flow rate and closed to increase the pressure and reduce the flow rate. The throttle valve is located at the exit to the outlet manifold (see Figure 3.17).

3.1.2.3 Test Gas Flow System

The test gas flow system (see Figure 3.19) is composed of a one or more K bottles (up to three), flow rate controller(s), throttle valve, pressure gauge, and vacuum pump. The gas flow from the K bottles is controlled by one or more MKS Instruments, Inc. electronic gas flow controllers (Model # 1259C-00100SV) depending on the type of test gas and the desired flow rate. 1/4" nylon tubing carries the test gas from the flow controller(s) to the test gas inlet(s) on the cathode housing of the cascade arc apparatus. After passing through the
Figure 3.19 Diagram of the test gas flow system.
cascade constrictor, the test gas exits in the anode housing and travels through the nylon tubing to a throttle valve. The throttle valve is adjusted to obtain the desired pressure in the cascade arc constrictor. This pressure is measured using the pressure gauge upstream of the throttle valve. The test gas is pumped from the system using a 5 cubic feet per minute mechanical vacuum pump located downstream of the throttle valve. The mechanical vacuum pump is a Duo Seal Vacuum Pump made by The Welch Co.

3.1.2.4 Translation System

The cascade arc assembly is attached to a translation table that has one degree of freedom. The table is positioned using a stepping motor with a 20,000 steps/in stepsize that allows accurate positioning of the cascade arc in the external optics (see Section 3.1.3). The translation table also allows the cascade to be moved out of the external optics while light sources for system calibration are positioned.

3.1.3 Optical System

Accurate measurement of plasma parameters requires careful integration of the optical design with the design of the central window section. To provide a small entrance solid angle for the cascade window section and to avoid off-axis aberrations, an adjustable, reflective Cassegrain optical collection system (telescope) is used. This collection system is on-axis to reduce spherical aberrations and has first surface mirrors to avoid chromatic aberrations. It collects light from the arc and directs it into a spectrometer so that the primary mirror in the spectrometer is overfilled (Figure 3.20). This ensures that the spectrometer grating is the limiting aperture in the optical system. The spectrometer has a focal length of 1.25 m and
utilizes a 316 groove/mm Echelle diffraction grating. This results in a linear dispersion of 25.1 Angstroms/mm in the first order. Before entering the Cassegrain telescope the light from the arc is rotated ninety degrees so that the radial dimension of the arc image lies along the entrance slit of the spectrometer. A two-dimensional optical multichannel analyzer (OMA) with image intensifier is used to collect and digitize the data. This detector has a 512 x 512 pixel detector array with 19 µm pixel spacing and is used to simultaneously acquire spectral data at many radial locations. Because the image of the arc is rotated ninety degrees before entering the spectrometer, the image collected by the 2-D OMA detector varies spectrally along each row and spatially along each column of the detector's pixel array. The magnification of the optical system is approximately 1.0 giving 200 spatial pixels across the 4 mm diameter arc channel. A picture of the optical setup using the OMA detector is shown in Figure 3.21.
Figure 3.21 Picture of the UTSI Cascade Arc Facility and external optics.
3.2 Experimental Procedure

The experimental procedure consists of two phases: system calibration and data acquisition. System calibration is necessary to obtain reliable data. The steps in the calibration procedure are presented in Section 3.2.1. The test procedure is discussed in Section 3.2.2. Because the UTSI Cascade Arc Facility has several subsystems that need to be operated manually during data acquisition, a brief discussion of the control of these systems is included in Section 3.2.2.

3.2.1 System Calibration

Wavelength calibration is performed on the spectral pixels using atomic lines from a low density helium calibration source. The spatial pixels were calibrated by taking images of a 50 μm vertical slit backlit by a continuous source and placed in the same position as the arc when the cascade is in operation. By moving the vertical slit across the location of the arc with a translation table, the spatial pixels were associated with a radial position across the arc region.

To determine the instrument broadening, or slit function of the spectrometer, images of the Ne 650.65 nm line from a standard, low pressure mercury vapor lamp were collected. The spectral lines from this standard lamp are essentially impulse functions because line broadening is insignificant at the low gas pressure in the lamp. By measuring the apparent line width of the line from the standard lamp, the slit function of the spectrometer can be determined. The slit function is necessary for correct interpretation of the spectral intensity data collected from the arc in the cascade. System calibration is performed before and after each data acquisition to ensure that the experimental setup has not changed. Details of data analysis are presented in Chapter 5.
3.2.2 Test Procedure

At least two persons must be present during data acquisition, one to monitor and control the cascade arc, and the other to acquire spectral data. The person responsible for data acquisition must control the spectrometer and operate the data acquisition equipment. The position of the optical components is not changed during the test.

Once the arc in the cascade is started, the control of the electrical power subsystem, the test gas flow subsystem, and the water cooling subsystem are all automated. The person responsible for running the cascade facility need only monitor these subsystems to insure proper operation. The gas pressure in the cascade constrictor may occasionally need adjustment by tweaking the throttle valve on the test gas flow subsystem. The cascade arc facility operator is also responsible for recording the arc current (fixed), the arc voltage, the potential of every constrictor plate, the constrictor pressure, the flow rate of the cooling water, and the temperature reading at every thermocouple location.

Operation of the cascade arc facility is complicated because several subsystems must function properly for steady state operation of the arc. A detailed list of the steps necessary to start, operate, and turn off the cascade arc is given in Appendix B.
CHAPTER 4

NUMERICAL SIMULATION RESULTS

The UTSI Cascade Arc Plasma Simulation (CAPS) code was used to simulate the UTSI Cascade Arc with hydrogen as a test gas. Simulations were run at pressures of 2.0 psi and 6.0 psi to match experimental conditions. The CAPS code was run with several different finite rate chemical kinetic models that have been used in the various arcjet simulation codes mentioned in Chapter 1. Simulation results and model comparisons are presented in this chapter.

4.1 CAPS Code Input Parameters and Convergence

The CAPS code requires two kinds of input parameters--program control parameters and physical parameters that describe geometry and plasma conditions. The physical parameters, shown in Table 4.1, were set equal to the experimental values used in the hydrogen arc experiment described in Chapter 5. The solution is highly sensitive to the current and pressure, but is relatively insensitive to the mass flow rate. Changing the mass flow rate by plus or minus an order of magnitude around the experimental value results in insignificant changes in the solution. This insensitivity to the mass flow rate is caused by the low gas velocity that leads to insignificant viscous heating. The wall temperature was assumed to be 300 K because the constrictor plates are water cooled. The heat transfer analysis discussed in Chapter 3 resulted in a predicted constrictor wall temperature of approximately
Table 4.1 Physical input parameters used in the CAPS code.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Code value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass flow rate [kg/sec]</td>
<td>$1.4 \times 10^{-8}$</td>
</tr>
<tr>
<td>Pressure [Pa]</td>
<td>$1.4 \times 10^4$ (2.0 psi)</td>
</tr>
<tr>
<td></td>
<td>or</td>
</tr>
<tr>
<td></td>
<td>$4.2 \times 10^4$ (6.0 psi)</td>
</tr>
<tr>
<td>Current [A]</td>
<td>50.0</td>
</tr>
<tr>
<td>Wall temperature [K]</td>
<td>300.0</td>
</tr>
</tbody>
</table>

500 K. However, the real wall temperature is unknown but is expected to be substantially lower than this upper limit because of the factors of safety and simplifying assumptions present in the heat transfer analysis. In any event, the simulation results are extremely insensitive to the wall temperature. Increasing the wall temperature to 900 K changed the simulated axial electric field and plasma power less than 0.3 percent and the centerline electron number density less than 5.0 percent. A 500 K wall temperature changed these values less than 0.2 percent and 1.8 percent, respectively. Therefore, the 300 K wall temperature assumed in the simulations is not believed to have significant effects on the comparisons with experimentally determined electron number densities and axial electric fields (see Chapters 5 and 6).

The computation grid used in the simulations is shown in Figure 4.1. This grid has 30 cells in the radial direction that are defined by 31 grid points. The grid points are spaced closer together as the wall is approached. This allows better
The computation grid used in the UTSI Cascade Arc Facility simulations is shown in Figure 4.1. It resolves steep gradients in the plasma near the wall and allows for better code convergence. The computation grid is discussed in greater detail in Chapter 2.

The program control parameters tell the CAPS code whether the simulation is to be equilibrium or nonequilibrium, define the convergence criterion, and give values for the under-relaxation parameters. The under-relaxation parameters are used to relax new values for dependent variables into the solution (see Chapter 2 for more details)—0.35 is a typical value.

The convergence criterion used by the code to check for convergence was arbitrarily set to $1 \times 10^{-11}$. Once the sum of the squares of all the residual errors drops below this value, the solution is no longer changing, and the CAPS code automatically stops. In the simulations presented in this chapter, the code was not run until this convergence criterion was met. The code was manually stopped when the solutions were no longer changing significantly over thousands of iterations (the sum of the squares of the residual errors would reduce by about an order of magnitude).
during these iterations. An additional criterion was used to determine simulation convergence. For a solution to be converged, it must satisfy the energy balance—the electrical power deposited into the plasma must equal the sum of the thermal conduction and optically thin radiation to the wall. Therefore, the CAPS code was also run until the energy balance was satisfied. At this point, the sum of the square of the residual errors was typically below $1 \times 10^{-9}$.

4.2 Description of the Kinetic Models

The CAPS code was run with several different finite rate chemical kinetic models to determine the effects of the kinetics on the solution. This section describes the various chemical kinetics models that have been used in the arcjet simulation codes mentioned in Chapter 1. The results from these simulations are presented and evaluated in Section 4.3.

4.2.1 'Equilibrium' Model

The rate constants are infinite in this model; therefore, all reactions are complete at the local pressure and temperature. As a result, the plasma species concentrations are determined using the Saha equation—a form of the law of mass action. See Chapter 2 for more details on the equilibrium modeling.
### 4.2.2 'Slow' Nonequilibrium Kinetics

The 'Slow' nonequilibrium kinetics solution models the interactions in the four-component hydrogen system using the reactions in Table 4.2 (M represents any non-electron third body). The forward reaction rate is computed using the rate coefficients in Table 4.2 in the Arrhenius equation (equation (2.14) repeated here for convenience).

\[ k_f = AT^{-n} \exp\left(\frac{E}{RT}\right) \]  

(4.1)

where

- **A** = Arrhenius constant
- **E** = activation energy
- **R** = universal gas constant
- **T** = absolute temperature.

The backward kinetic reaction rate coefficients, \( k_b \), are calculated from \( k_f \) and the equilibrium constant, \( K_p \) (equation (2.15) repeated here for convenience).

\[ k_b = -\frac{k_f}{K_p} \]  

(4.2)

All of the rate coefficients shown in Table 4.2, except for two, were taken from McCay et al. [85]. The first exception is the slight modification of the recombination rate of atomic hydrogen to fit data from Park [60]. The second exception is the rate of ionization of atomic hydrogen by electrons. This rate was calculated from cross-section data [86] using methods presented by Keefer [87]. According to Keefer, ionization can occur in a two-step process where an atom that has already been excited by an electron is ionized by a collision with a second electron. The
Table 4.2 Reactions and rate constants used in the 'Slow' nonequilibrium model.

<table>
<thead>
<tr>
<th></th>
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<th></th>
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<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$H + H + M \leftrightarrow H_2 + M$</td>
<td>6.40e+17</td>
<td>$T_H$</td>
<td>1.0</td>
<td>0.</td>
</tr>
<tr>
<td>2</td>
<td>$H^+ + e + M \leftrightarrow H + M$</td>
<td>5.26e+26</td>
<td>$T_H$</td>
<td>2.5</td>
<td>0.</td>
</tr>
<tr>
<td>3</td>
<td>$H_2 + e \rightarrow H + H + e$</td>
<td>1.91e+11</td>
<td>$T_e$</td>
<td>-1.0</td>
<td>-203.</td>
</tr>
<tr>
<td>4</td>
<td>$H^+ + e \rightarrow H + hv$</td>
<td>3.77e+13</td>
<td>$T_e$</td>
<td>0.58</td>
<td>0.</td>
</tr>
<tr>
<td>5</td>
<td>$H^+ + e + e \rightarrow H + e$</td>
<td>2.19e+41</td>
<td>$T_e$</td>
<td>5.06</td>
<td>0.</td>
</tr>
<tr>
<td>6</td>
<td>$H + e \rightarrow H^+ + e + e$</td>
<td>1.81e+14</td>
<td>$T_e$</td>
<td>0.</td>
<td>-244750</td>
</tr>
</tbody>
</table>

Source:

ionization of the excited atom will be faster than the excitation process itself because the ionization of the excited atom requires less energy. To incorporate this effect into the CAPS code kinetics model without introducing a new species--excited atomic hydrogen--the collision cross-section was modified to equal zero at the excitation potential of 10.2 eV rather than at the ionization potential of 13.4 eV [54]. The resulting reaction rate was fitted to the Arrhenius equation and gives the results shown in Table 4.2.
4.2.3 'Fast' Nonequilibrium Kinetics

The 'Fast' nonequilibrium kinetics model was presented by Rhodes et. al. [54]. The reaction rate coefficients for these reactions are the same as for the 'Slow' nonequilibrium kinetics, except the recombination rate of atomic hydrogen (reaction number 5 in Table 4.2) is calculated by substituting the forward rate for ionization (reaction number 6 in Table 4.2) and the equilibrium constant into equation (4.2).

The 'Fast' nonequilibrium reaction set is shown in Table 4.3.

4.2.4 'University of Illinois (U of I)' Nonequilibrium Kinetics

The 'U of I' nonequilibrium reaction set is exactly the same as the 'fast' nonequilibrium set, and all of the rate coefficients are the same except for one. The 'U of I' model has a different kinetic rate coefficient for the dissociation of diatomic

Table 4.3 Reactions and rate constants used in the 'Fast' nonequilibrium model.

<table>
<thead>
<tr>
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<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>H + H + M ↔ H2 + M</td>
<td>6.40e+17</td>
<td>TH</td>
<td>1.0</td>
<td>0.</td>
</tr>
<tr>
<td>2</td>
<td>H^+ + e + M ↔ H + M</td>
<td>5.26e+26</td>
<td>TH</td>
<td>2.5</td>
<td>0.</td>
</tr>
<tr>
<td>3</td>
<td>H2 + e → H + H + e</td>
<td>1.91e+11</td>
<td>Te</td>
<td>-1.0</td>
<td>-203.</td>
</tr>
<tr>
<td>4</td>
<td>H^+ + e → H + hv</td>
<td>3.77e+13</td>
<td>Te</td>
<td>0.58</td>
<td>0.</td>
</tr>
<tr>
<td>5</td>
<td>H^+ + e + e ↔ H + e</td>
<td>7.08e+39</td>
<td>Te</td>
<td>4.5</td>
<td>0.</td>
</tr>
</tbody>
</table>

Source:
hydrogen by electrons (reaction number 3 in Table 4.3) [5]. This dissociation rate
data, presented by Janev et. al. [88], was fitted to the Arrhenius equation for electron
energies up to 1 eV. The fitted curve is utilized in the CAPS code 'U of I' reaction
set. The maximum electron temperature realized in the 'U of I' simulations remained
below 1 eV (discussed in Section 4.3.3). The 'U of I' reaction set and the rate
coefficients used in the CAPS code are shown in Table 4.4.

4.2.5 'Fast' Nonequilibrium Kinetics with a Reflective Wall

All of the kinetics models presented above assume a catalytic boundary
condition. At a catalytic wall, all reactions are complete. Therefore, at the assumed
300 K wall temperature, recombination of ions and atomic hydrogen are complete.
This is not true for the 'Fast' nonequilibrium kinetics model with a reflective wall. It

Table 4.4 Reactions and rate constants used in the 'U of I' nonequilibrium model.

<table>
<thead>
<tr>
<th></th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>H + H + M ↔ H₂ + M</td>
<td>6.40e+17</td>
<td>T_H</td>
<td>1.0</td>
<td>0.</td>
</tr>
<tr>
<td>2</td>
<td>H⁺ + e + M ↔ H + M</td>
<td>5.26e+26</td>
<td>T_H</td>
<td>2.5</td>
<td>0.</td>
</tr>
<tr>
<td>3</td>
<td>H₂ + e → H + H + e</td>
<td>1.87e-3</td>
<td>T_e</td>
<td>-3.73</td>
<td>0.</td>
</tr>
<tr>
<td>4</td>
<td>H⁺ + e → H + hv</td>
<td>3.77e+13</td>
<td>T_e</td>
<td>0.58</td>
<td>0.</td>
</tr>
<tr>
<td>5</td>
<td>H⁺ + e + e ↔ H + e</td>
<td>7.08e+39</td>
<td>T_e</td>
<td>4.5</td>
<td>0.</td>
</tr>
</tbody>
</table>

Source:
T. Megli, H. Krier, and R. Burton, "A Plasmadynamics Model for
Nonequilibrium Processes in N₂/H₂ Arcjets," AIAA 95-1961, 26th AIAA
has the same reaction rates as the 'Fast' nonequilibrium model, but assumes a reflective wall boundary condition [89].

The reflective wall boundary condition assumes that the plasma species are reflected off of the wall (Neumann boundary condition). This increases the electron number densities near the wall and leads to an increased electron number density throughout the entire system. Since the wall is non-catalytic, the reactions at the wall are not assumed to be complete as in the other simulations. It is important to note that this reflective wall boundary condition was selected as a limiting case to investigate the influence of the wall boundary conditions on simulated species concentrations—not as an attempt to model realistic plasma behavior.

### 4.3 Simulation Comparisons

The finite rate chemical kinetic models have a large impact on the plasma properties. Large variations in temperature, species concentrations, and plasma energy are seen between the model solutions. These variations are presented and discussed in this section.

#### 4.3.1 Comparison of Predicted Mole Fractions

The predicted mole fractions vary significantly from one finite rate chemical kinetics model to the next. Radial distributions of the mole fractions of the species for the equilibrium solutions appear in Figures 4.2 and 4.3 for pressures of 2.0 psi and 6.0 psi, respectively. For these cases, the plasma is approximately ten percent ionized on the centerline. The concentration of atoms decreases and the concentration of
Figure 4.2 Radial distribution of species mole fractions for the equilibrium simulation of a 50 A hydrogen arc at a pressure of 2 psi.

Figure 4.3 Radial distribution of species mole fractions for the equilibrium simulation of a 50 A hydrogen arc at a pressure of 6 psi.
diatomic hydrogen increases quite rapidly beyond a radius of 1.25 mm. As expected, the electron population decreases at the same time. All of the electrons are essentially recombined beyond a radius of 1.5 mm.

The 'Slow' nonequilibrium model results in the predicted mole fractions shown in Figures 4.4 and 4.5 for the 2.0 psi and the 6.0 psi cases, respectively. For these cases, the ionization fraction at the centerline is as high as an order of magnitude smaller than for the equilibrium model. Unlike the equilibrium model, however, the ionization fraction for the 'Slow' nonequilibrium cases remains significantly high until very close to the catalytic wall. This occurs because the electrons near the center of the arc diffuse toward the wall in a length of time too short for chemical equilibrium to be complete. Diffusion also leads to larger concentrations of molecular hydrogen in the arc core for the nonequilibrium model.

Figures 4.6 and 4.7 show the radial distribution of mole fractions for the 'Fast' nonequilibrium simulations. These 'Fast' simulation results have the same trends as the 'Slow' simulation results, but have higher ionization fractions. The ionization fraction for the 6.0 psi case is slightly higher than the 2.0 psi case. This occurs because more collisions take place at higher pressures.

The results from the 'U of I' simulations have a drastically different composition when compared to the other nonequilibrium models discussed above (see Figures 4.8 and 4.9). The dissociation rate of diatomic hydrogen by electrons is much slower for the 'U of I' reaction set used in the simulations. Therefore, diatomic hydrogen has a much larger mole fraction for this reaction set than is seen with the other finite rate chemical kinetics models. At 2.0 psi (Figure 4.8), the centerline mole fraction of diatomic hydrogen actually exceeds the mole fraction of hydrogen. The

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Figure 4.4 Radial distribution of species mole fractions for the 'Slow' nonequilibrium simulation of a 50 A hydrogen arc at a pressure of 2 psi.

Figure 4.5 Radial distribution of species mole fractions for the 'Slow' nonequilibrium simulation of a 50 A hydrogen arc at a pressure of 6 psi.
Figure 4.6 Radial distribution of species mole fractions for the 'Fast' nonequilibrium simulation of a 50 A hydrogen arc at a pressure of 2 psi.

Figure 4.7 Radial distribution of species mole fractions for the 'Fast' nonequilibrium simulation of a 50 A hydrogen arc at a pressure of 6 psi.
Figure 4.8 Radial distribution of species mole fractions for the 'U of I' nonequilibrium simulation of a 50 A hydrogen arc at a pressure of 2 psi.

Figure 4.9 Radial distribution of species mole fractions for the 'U of I' nonequilibrium simulation of a 50 A hydrogen arc at a pressure of 6 psi.
ionization fractions predicted by the 'U of I' model, however, are similar to the ionization fraction predicted by the other nonequilibrium models.

The radial distributions of mole fractions predicted by the 'Fast' nonequilibrium model with reflective walls appear in Figures 4.10 and 4.11 for the 2.0 psi case and 6.0 psi case, respectively. Unlike all of the other nonequilibrium simulations that assume a catalytic wall, the mole fraction of atomic hydrogen remains nearly constant all the way to the wall. The centerline ionization fraction is similar to that predicted by the 'U of I' model at both pressures.

4.3.2 Comparison of Predicted Velocities

The axial velocity realized in the cascade arc constrictor is very small. This small velocity leads to insignificant axial gradients in a cascade arc simulation and makes the cascade arc a good tool for studying plasmas (see Chapter 2). The radial distributions of the axial velocities for the CAPS code simulations are shown in Figures 4.12 and 4.13 for the 2.0 psi and 6.0 psi cases, respectively. The predicted velocities are all under 9 m/s, and the simulated velocities at 2.0 psi are about half their respective values in the 6.0 psi simulation.

Assuming a perfect gas, the axial velocity, \( u \), can be shown to be directly proportional to the gas temperature, \( T \).

\[
\mathbf{u} = \left( \frac{\dot{m} R}{PA} \right) \cdot T \tag{4.4}
\]

where

\( \dot{m} = \) the mass flow rate,
\( R = \) the gas constant,
Figure 4.10 Radial distribution of species mole fractions for the 'Fast' nonequilibrium simulation of a 50 A hydrogen arc at a pressure of 2 psi with a reflective wall.

Figure 4.11 Radial distribution of species mole fractions for the 'Fast' nonequilibrium simulation of a 50 A hydrogen arc at a pressure of 6 psi with a reflective wall.
Figure 4.12 Radial distributions of axial velocity for the 50 A hydrogen arc simulations at 2.0 psi.

Figure 4.13 Radial distributions of axial velocity for the 50 A hydrogen arc simulations at 6.0 psi.
\[ P = \text{the pressure, and} \]
\[ A = \text{the area of the constrictor cross-section.} \]

The temperature coefficient (the leading term in parenthesis in equation (4.4)) is constant along the constrictor axis in a cascade arc. Since the mass flow rate and cross-section of the constrictor are constant for all cases, the temperatures realized at the higher pressure should be higher than at the lower pressure. This anticipated result is confirmed in Section 4.3.3.

### 4.3.3 Comparison of Predicted Temperatures

Comparisons of the radial temperature distributions for the equilibrium and the 'Slow' nonequilibrium cases are located in Figure 4.14 for the 2.0 psi simulations and in Figure 4.15 for the 6.0 psi simulations. The electron temperature is much higher than the heavy particle temperature. The large difference between the electron temperature and the heavy particle temperature shown in these figures indicates a significant departure from thermal equilibrium. At 6.0 psi, more collisions occur between the electrons and heavy particles. Therefore, the electron temperature at 6.0 psi is lower than in the 2.0 psi case, and the solution is somewhat closer to equilibrium. The equilibrium temperature distribution is more closely matched by the heavy particle temperature, as expected. Near the wall, electrons lose so much energy acting as a third body in reactions with diatomic hydrogen that the electron temperature drops below the heavy particle temperature. This feature is present at both pressures but is more pronounced at 6.0 psi.
Figure 4.14 Radial temperature distribution of the heavy particle and electron temperatures in the 'Slow' nonequilibrium solution of a 50 A hydrogen arc at 2.0 psi. The equilibrium solution is shown as a baseline.

Figure 4.15 Radial temperature distribution of the heavy particle and electron temperatures in the 'Slow' nonequilibrium solution of a 50 A hydrogen arc at 6.0 psi. The equilibrium solution is shown as a baseline.
The radial temperature distributions for the 'Fast' nonequilibrium model at 2.0 psi and 6.0 psi can be seen, respectively, in Figures 4.16 and 4.17. The higher ionization rate by electrons realized in the 'Fast' model results in a greater number of electrons which can collide with atoms. Through increased collisions, the electrons lose more thermal energy to the heavy particles than in the 'Slow' model solution. This process brings the electron temperature and the heavy particle temperature closer together in the 'Fast' case. Because more collisions occur at higher pressures, the 6.0 psi case is significantly closer to thermal equilibrium than the 2.0 psi case. Given enough collisions, the nonequilibrium plasma would eventually reach thermal equilibrium. The equilibrium temperature profiles are shown in Figures 4.16 and 4.17 for reference. As in the 'Slow' model, the 'Fast' model results in electron temperature profiles that drop below the heavy particle temperature near the wall. This effect is amplified in the 'Fast' solutions because they have a greater degree of ionization (see Figures 4.4 through 4.7). Thus, more atomic hydrogen must recombine at the wall in the 'Fast' case than in the 'Slow' case causing a lower electron temperature.

Figures 4.18 and 4.19 show the radial temperature profiles realized from the 'U of I' finite rate chemical kinetics model at 2.0 psi and 6.0 psi, respectively. The peak temperature is lower than in the 'Slow' and 'Fast' solutions. As in the other nonequilibrium models, the 'U of I' model results in the 6.0 psi case being closer to thermal equilibrium than the 2.0 psi case. Unlike the other nonequilibrium models, the electron temperature does not drop below the heavy particle temperature near the wall in the 'U of I' model solutions. This occurs because the plasma in the 'U of I' simulations is not as highly dissociated or ionized, and therefore takes less thermal energy from the electron gas during recombination at the wall.
Figure 4.16 Radial temperature distribution of the heavy particle and electron temperatures in the 'Fast' nonequilibrium solution of a 50 A hydrogen arc at 2.0 psi. The equilibrium solution is shown as a baseline.

Figure 4.17 Radial temperature distribution of the heavy particle and electron temperatures in the 'Fast' nonequilibrium solution of a 50 A hydrogen arc at 6.0 psi. The equilibrium solution is shown as a baseline.
Figure 4.18 Radial temperature distribution of the heavy particle and electron temperatures in the 'U of I' nonequilibrium solution of a 50 A hydrogen arc at 2.0 psi. The equilibrium solution is shown as a baseline.

Figure 4.19 Radial temperature distribution of the heavy particle and electron temperatures in the 'U of I' nonequilibrium solution of a 50 A hydrogen arc at 6.0 psi. The equilibrium solution is shown as a baseline.
The temperature distributions for the 'Fast' finite rate chemistry model solutions with reflective walls (Figures 4.20 and 4.21) are very similar to the 'U of I' temperature distributions (Figures 4.18 and 4.19). Both the peak temperatures and the profiles are comparable. In the 'Fast' reflective wall simulations, the electron temperature remains above the heavy particle temperature near the wall because the reflective wall does not force recombination of all of the atoms. (Recombination at the wall is low for the 'U of I' case because of a small mole fraction of atomic hydrogen, not because a reflective wall prevents recombination.)

4.3.4 Comparison of Predicted Electrical Conductivities

The electrical conductivity is a very important property to know when modeling a plasma since it is used to determine the electrical power input. Figure 4.22 is a plot of the radial distribution of electrical conductivity for all the simulations at 2.0 psi. The same plot is shown in Figure 4.23 for 6.0 psi. Differences in the nonequilibrium electrical conductivities vary as much as 250 percent at 2.0 psi and 200 percent at 6.0 psi. The profiles are comparable at both pressures, but the electrical conductivities are slightly higher on the centerline for the 6.0 psi case. It is important to note that the equilibrium electrical conductivity is essentially zero beyond a radius of 1.25 mm because of a lack of electrons in this region. The nonequilibrium electrical conductivity has a significant value all the way to the wall because electrons do exist this area as a result of chemical nonequilibrium.
Figure 4.20 Radial temperature distribution of the heavy particle and electron temperatures in the 'Fast' nonequilibrium solution of a 50 A hydrogen arc at 2.0 psi with reflective walls. The equilibrium solution is shown as a baseline.

Figure 4.21 Radial temperature distribution of the heavy particle and electron temperatures in the 'Fast' nonequilibrium solution of a 50 A hydrogen arc at 6.0 psi with reflective walls. The equilibrium solution is shown as a baseline.
Figure 4.22 Radial distributions of electrical conductivity for the 50 A hydrogen arc simulations at 2.0 psi.

Figure 4.23 Radial distributions of electrical conductivity for the 50 A hydrogen arc simulations at 6.0 psi.
4.3.5 **Energy Balance Comparisons**

As stated in Section 4.1, the CAPS code is not considered converged until the energy balance is satisfied. Therefore, the electrical power deposited into the plasma must equal losses at the wall. The energy balance--power balance for our purpose--for the solution to each finite rate chemical kinetics model is presented in this subsection.

The electrical power, \( P_{\text{electric}} \), deposited into the plasma is calculated using

\[
P_{\text{electric}} = 2\pi E^2 \int_0^{r_{\text{wall}}} \sigma r \, dr
\]

(4.5)

where

\( E = \) the electric field,

\( \sigma = \) the electrical conductivity,

\( r_{\text{wall}} = \) the radius of the constrictor wall;

and the electric field, \( E \), is calculated from

\[
E = \frac{I}{2\pi \int_0^{r_{\text{wall}}} \sigma r \, dr}
\]

(4.6)

where \( I \) is the current. The electrical power input to the plasma and the electric field are strongly dependent on the electrical conductivity of the plasma. The range of predicted electrical conductivities discussed in Section 4.3.2 can result in significant changes in the predicted plasma power. Tables 4.5 and 4.6 show the energy balance and electric field for each solution of the various finite rate chemical kinetic models at 2.0 psi and 6.0 psi, respectively. In these tables, the Power In column is calculated
Table 4.5 Power balance for the CAPS code simulations of a 50 A hydrogen arc at 2.0 psi.

<table>
<thead>
<tr>
<th>Chemical Kinetics Model</th>
<th>Electric Field [V/cm]</th>
<th>Power In [Watts/cm]</th>
<th>Power Out [Watts/cm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Equilibrium</td>
<td>46.4</td>
<td>2320.</td>
<td>2264.</td>
</tr>
<tr>
<td>'Slow' Non-equilibrium</td>
<td>95.7</td>
<td>4785.</td>
<td>4707.</td>
</tr>
<tr>
<td>'Fast' Non-equilibrium</td>
<td>42.0</td>
<td>2099</td>
<td>2075</td>
</tr>
<tr>
<td>'U of I' Non-equilibrium</td>
<td>33.4</td>
<td>1670.</td>
<td>1676.</td>
</tr>
<tr>
<td>'Fast' Non-equilibrium with Reflective Walls</td>
<td>36.4</td>
<td>1821.</td>
<td>1795.</td>
</tr>
</tbody>
</table>
Table 4.6 Power balance for the CAPS code simulations of a 50 A hydrogen arc at 6.0 psi.

<table>
<thead>
<tr>
<th>Chemical Kinetics Model</th>
<th>Electric Field [V/cm]</th>
<th>Power In [Watts/cm]</th>
<th>Power Out [Watts/cm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Equilibrium</td>
<td>46.3</td>
<td>2317.</td>
<td>2267</td>
</tr>
<tr>
<td>'Slow' Non-equilibrium</td>
<td>64.9</td>
<td>3245.</td>
<td>3178.</td>
</tr>
<tr>
<td>'Fast' Non-equilibrium</td>
<td>43.9</td>
<td>2195.</td>
<td>2179.</td>
</tr>
<tr>
<td>'U of I' Non-equilibrium</td>
<td>44.1</td>
<td>2205.</td>
<td>2223.</td>
</tr>
<tr>
<td>'Fast' Non-equilibrium with Reflective Walls</td>
<td>36.9</td>
<td>1844.</td>
<td>1850.</td>
</tr>
</tbody>
</table>
using equation (4.5). The Power Out column is the energy loss at the wall. In general, wall losses include both thermal conductivity to the wall and optically thin radiation to the wall. Since the optically thin radiation contributes insignificant wall losses, the losses are set equal to the thermal conduction at the wall. The wall losses are calculated using

$$\frac{dT}{dr} = 2\pi r_{wall} k_{th} \left. \frac{dT}{dr} \right|_{r=r_{wall}}$$

(4.7)

where $k_{th}$ is the thermal conductivity.

The maximum discrepancies between the ‘Power In’ and ‘Power Out’ columns is 2.47 percent at 2.0 psi and 2.11 percent at 6.0 psi. This maximum error occurs for the equilibrium solution for both pressures. The rest of the solutions have better convergence, with power balance errors typically less than one percent. The plasma power predicted by the different kinetics models varies by more than 3.0 kilowatts/cm for the 2.0 psi case and 1.3 kilowatts/cm for the 6.0 psi case. The simulations with lower electrical conductivity result in higher power input (see Figures 4.22 and 4.23 and Tables 4.5 and 4.6). This result is expected since the substitution of equation (4.6) into equation (4.5) shows power to be inversely proportional to electrical conductivity. The plasma powers listed in Tables 4.5 and 4.6 will be compared to experimental values in Chapter 6.
EXPERIMENTAL DATA ANALYSIS

The cascade arc was operated with pure hydrogen arcs at 2.0 psi and 6.0 psi and a current of 50 A. By using hydrogen and nitrogen mixtures with the correct mixture ratios, simulated ammonia and hydrazine arcs at 2.0 psi, 6.0 psi, and 10.0 psi were also run at a current of 50 A. Spectral emission data from the 656.28 nm Balmer alpha, $H_\alpha$, line were collected using a 1.25 m Spex spectrometer with a 316 groove/mm Echelle grating operated in the eighth order and a two-dimensional OMA detector [64]. Nine images of the arc were collected at each pressure for hydrogen, and three images were collected at each pressure for the hydrogen/nitrogen mixture. A 1.9 N.D. filter and a 550 nm high-pass filter were utilized to prevent detector saturation and eliminate interference from higher order lines, respectively. For the hydrogen plasmas, the OMA detector exposure times were 0.2 seconds for the 6.0 psi case and 2.0 seconds for the 2.0 psi case. The 2.0 psi case required longer exposure times because the intensity of the radiation was lower. The exposure times for the simulated ammonia and hydrazine plasmas were 2.0, 5.0, and 10 seconds for the 10 psi, 6 psi, and 2 psi cases, respectively. Longer exposure times were necessary because the mixture plasmas were less intense than the hydrogen plasmas. The images of the arcs are composed of 512 spectral pixels and 400 spatial pixels. Wavelength calibration (fully described in Chapter 3) was performed on the spectral pixels using lines from a low-density neon calibration source. The spatial pixels were calibrated by taking images of a 50 µm vertical slit backlit by the neon lamp and
placed in the same position as the arc when the cascade is in operation. By moving the vertical slit across the location of the arc with a precision translation table, the spatial pixels were associated with a radial position across the arc region. The spectrometer slit function was experimentally measured using a narrow neon spectral line, and the measured spectral lines were spectrally deconvolved using a digital Wiener filter [90].

The spatially resolved Hα line data was utilized to determine the radial distribution of electron number density of the plasmas in the cascade arc. The axial electric fields have been experimentally determined. Rough estimates of the electron temperatures were also established. These electron temperature, electric field, and number density data were not measured directly; they result from processing the raw data. This chapter presents details of the steps required to calculate these quantities from raw data collected during operation of the cascade arc. Figure 5.1 presents an overview of the experimental data analysis procedure, including corresponding chapter section numbers for each step. Results of the data analysis are discussed in Chapter 6.

5.1 Determination of the Axial Electric Field

The axial electric field is the spatial derivative of the plasma potential along the length of the arc. As described in detail in Chapter 3, the electric arc is stabilized by the constrictor wall in the UTSI cascade arc. This constrictor is comprised of a series of electrically isolated copper plates that are stacked together. Because the copper plates are electrically isolated from each other, they will have an electric potential equal to the potential of the electric arc passing through them. Therefore,
Figure 5.1 Experimental data analysis procedure.
the plasma potential can be determined by measuring the potentials of the constrictor plates during operation of the cascade arc. A voltmeter with hand-held probes was used to collect this data.

The electric field was determined by plotting the electric potential of each of the constrictor plates versus the corresponding positions of the plates. The electric field and the uncertainty of the electric field are equal to the slope and the uncertainty of the slope of the best fit line through the data points, respectively. Figure 5.2 is an example plot used to determine the electric field for a 50 A hydrogen arc at 6.0 psi. The equation for the best fit line and the slope uncertainty are shown in the caption of this figure. It is important to note that the first and last potentials correspond to electrode potentials (not shown in Figure 5.2) and were not utilized in the linear regression. These points were not considered because the exact positions of the electrodes in their housings cannot be measured with a high degree of accuracy.

Also, the electrodes have plasma sheaths associated with them. These sheaths contain a distribution of charged particles that electrically shield the plasma particles outside of the sheath from the electrodes. The negatively charged cathode is hidden by a positively charged sheath, and the positively charged anode is hidden by a negatively charged sheath. The potential changes a few volts in the very short distance (on the order of one Debye length—$10^{-6}$ to $10^{-7}$ m for the thermal plasmas seen in the cascade arc [9]) across typical plasma sheaths—leading to sheath electric fields significantly larger than those seen in the plasma. Therefore, including the potentials associated with the electrodes would result in an electric field that is too high to be indicative of the axial electric field at the window section (where comparisons with computer simulation are made).
Figure 5.2 Example plot of the electric potentials of the constrictor plates used to determine the electric field of a 50 A hydrogen arc at 6.0 psi. The "Best Fit Line" is the linear regression: Volts = 44.2 * Axial Position + 26.5; \( R^2 = 0.9957 \).
The power deposited into the cascade arc plasma is a function of the electric field. To perform a check on the electric field measurement, the power deposited into the plasma can be compared to the power carried out of the system by the cooling water. The power deposited into the plasma is given by:

\[ \text{Power in} = I \times E \]  

(5.1)

where

\[ I = \text{Arc current} = 50.2 \pm 0.1 \text{ A} \]

\[ E = \text{Electric field} \]

The power removed from the plasma by the cooling water is given by:

\[ \text{Power out} = V \times \rho \times C_p \times \frac{\Delta T}{L} \]  

(5.2)

where

\[ V = \text{volumetric flow rate} \]

\[ \rho = \text{density of cooling water} \]

\[ C_p = \text{specific heat of cooling water} \]

\[ \Delta T = \text{rise in cooling water temperature in window section} \]

\[ L = \text{Length of window section cooled by water channel.} \]

As is presented in Chapter 6, the power deposited into the plasma is the same as the power removed by the cooling water within experimental uncertainty, which is consistent with a correctly measured electric field.
5.2 Determination of the Radial Distribution of Electron Number Density

The radial distribution of electron number density is determined from analysis of the spatially resolved intensity of the hydrogen Balmer alpha, $\text{H}_\alpha$, line. Figure 5.3 shows a gray scale, 2-D OMA image of the $\text{H}_\alpha$ line intensity for a typical 50 A hydrogen arc. The intensity in this figure has been normalized to one. The wavelength varies along the abscissa and the radial position varies along the ordinate. The steps required to calculate the electron densities from the spatially resolved intensity data are discussed below.

5.2.1 Adjust Intensity Data Using Background and Spectral Shift

The first step in processing the spatially resolved intensity data is to subtract the background noise from the raw data. Signal from artificial lights and the dark noise associated with the 2-D OMA CCD camera are removed from the $\text{H}_\alpha$ line intensity in this step.

In a grating spectrometer, a constant wavelength source shifts to shorter wavelengths as one moves off axis (towards the top or bottom of the entrance slit). This curvature results in a bow-shaped line for a constant wavelength source [91]. The 1.25 m Spex Spectrometer used in the cascade arc experiment has a curved entrance slit to allow a greater slit height than would be possible with a straight slit. Therefore, the position of a constant wavelength in the focal plane (located at the OMA detector surface at the spectrometer's exit) moves to the left or right as one moves spatially off-axis in the focal plane. This effect is demonstrated in Figure 5.4 which contains a diagram of the focal plane at the exit of the spectrometer.
Figure 5.3  Spatially resolved, gray scale image of the $H\alpha$ line of a 50 A hydrogen arc at 6.0 psi.
Figure 5.4 Diagram showing the curvature of a constant wavelength in the focal plane of the 1.25 m Spex Spectrometer with curved entrance slit.
All images of the H\textsubscript{\alpha} line from the cascade arc plasma have this spatially dependent, spectral curvature which must be removed before further data reduction can take place. This is accomplished by shifting each spectral row a prescribed amount so that the same wavelengths in each spatial row in the image occupy the same spectral pixel.

5.2.2 Deconvolution of the Slit Function

After the background noise has been removed from the image of the H\textsubscript{\alpha} line, and the spectral shift of off-axis rows has been corrected, the instrument broadening due to the spectrometer entrance slit must be removed. This broadening mechanism--broadening due to the spectrometer slit function--is a result of the finite width of the entrance slit. The slit function is the response of the spectrometer to a source that is an impulse function (infinitesimally small width compared to the width of the slit). When sources with much broader line widths are focused onto the spectrometer entrance slit, the lineshape realized in the focal plane at the spectrometer exit is the convolution of the actual signal with the slit function [91].

The slit function can be measured by focusing the image of a standard, low pressure, neon vapor lamp onto the entrance slit of the spectrometer and recording the intensity from one of the atomic lines. Because the gas in the lamp is at a low pressure, the atomic lines emitted are not significantly broadened via collisions and have a much smaller width than the equivalent spectral width of the entrance slit. Therefore, an atomic spectral line from the low pressure lamp acts as an impulse function to the spectrometer, thus, allowing the slit function to be measured. The 1.25 m Spex spectrometer slit function was measured using the 650.65 nm line in the
spectrum of a standard, low pressure, neon lamp. This line was chosen because it is a strong line at a wavelength close to the 656.28 nm H\textsubscript{\alpha} line. The measurement was performed in the same spectral order as the measurement of the H\textsubscript{\alpha} line in the cascade experiment. This eliminates the possibility of any error that might be introduced from the determination of the slit function in a different order. Figure 5.5 shows an example of the measured slit function. The peak intensity of the slit function has been normalized to one.

To remove the influence of the slit function from the measured H\textsubscript{\alpha} line, a digital Wiener filter was used to deconvolve the measured slit function from the measured H\textsubscript{\alpha} line at each spatial location (each row—see Figure 5.2) of the 2-D OMA image. The digital Wiener filter has the form [90]:

\begin{equation}
F(u) = \left[ \frac{1}{H(u)} \frac{|H(u)|^2}{|H(u)|^2 + K} \right] G(u) \tag{5.3}
\end{equation}

where

\begin{align*}
H(u) &= \text{the discrete Fourier transform of the slit function,} \\
G(u) &= \text{the discrete Fourier transform of the signal convolved with the slit function} \\
F(u) &= \text{the discrete Fourier transform of the signal with the slit function removed} \\
u &= \text{frequency variable representing wavelength in the Fourier domain} \\
K &= \text{is a small, positive constant that prevents singularities in the event that intensity of the slit function at (u) is zero.}
\end{align*}
Figure 5.5 Slit function of the 1.25 m Spex spectrometer determined from the 650.65 nm line of a standard low pressure neon lamp.

The Wiener filter returns the Fourier transform of the signal, $F$, with the slit function deconvolved. Taking the discrete inverse Fourier transform of $F$ results in the non-Fourier transformed signal with all slit function effects removed. The FORTRAN code written to implement this deconvolution algorithm utilizes Fast Fourier Transforms (FFT's) to perform the deconvolution as quickly as possible. This deconvolution program was verified using, as input, the convolution of a user generated slit function and a user generated signal that have Gaussian profiles with known widths. The discrete Wiener filter algorithm was found to be very robust. During analysis of the cascade arc data, the constant, $K$, in equation (5.3) was set to 0.001. This value for $K$ was verified to result in no apparent degradation of the signal.
Significantly larger values of K have the tendency to artificially broaden the signal during deconvolution of the slit function.

5.2.3 Abel Inversion

The 2-D OMA captures spectral intensity data at many spatial locations across the arc simultaneously. Because this intensity data is a line-of-sight projection of the emission data onto a one-dimensional plane, it must be transformed, via Abel inversion, to obtain radial profiles of the spectral emission. Theoretical emission lines can then be compared to this radial distribution of spectral lines to determine the radial variation of electron number density (explained in detail in Section 5.2.4).

"The determination of a radially symmetric, two-dimensional function from its one dimensional projection is known as Abel inversion." [92] The Abel inversion assumes that the radially symmetric function can be comprised of N mutually concentric circles--each having constant value for the function (see Figure 5.6). The value of the projection of the function corresponding to the outer ring (ring N in Figure 5.6), along with the geometry of the outer ring, can be used to determine the value of the function for that ring (none of the inner rings contribute to the line of sight projection at this location). Once the function of the outer ring is determined, the value of the second ring from the outer edge, ring N-1, can be found. This is accomplished by taking the projection of the function corresponding to ring N-1 and subtracting the contribution due to ring N. The value of the function in ring N-2 can now be determined since the values of the outer rings are already known. By repeating this procedure, the radial distribution of the entire function can be obtained.
The Abel inversion of the 2-D OMA images is performed using a modern approach that utilizes integral transforms [92]. In this method, the Abel inversion of line-of-sight intensity data into radially distributed emission data is accomplished by taking the Fourier transform of the intensity data and then performing an inverse Hankel transform. A method for determining the center of the data that minimizes asymmetries is incorporated in this inversion technique. Because Abel inversion implies radial symmetry, any asymmetry is assumed to be noise. Since the Fourier transform of symmetric data is real and the Fourier transform of asymmetric data has imaginary components, the imaginary components of asymmetric data are noise, by definition. Therefore, by shifting the data so that the imaginary components of the transform are minimized, the center can be found. Because fast Fourier transforms
(FFT's) can be implemented in the method described above, this Abel inversion process can be performed much faster than conventional methods.

The following algorithm has been used to implement this Abel inversion approach in our data analysis. (1) A fast Fourier transform (FFT) is performed on the intensity data. (2) High frequency noise is filtered out of spectral data using an optimal, finite impulse response (FIR), low band pass filter. (3) The inverse fast Fourier transform (IFFT) is performed on the data. These first three steps smooth the spectral data by filtering out high frequency noise. The Abel inversion is performed next. (4) Perform the FFT on spatial data. (5) Filter the spatial high frequency noise using another optimal, FIR, low band pass filter. (6) Center the transformed data by shifting to minimize the imaginary component of transformed data. (7) Discard the imaginary part of the shifted, transformed data. This step eliminates noise (asymmetries) in the data. (8) Perform the inverse Hankel transform to obtain the Abel inverted data.

In order to implement the FFT Abel inversion technique on the cascade arc data, both the spectral and spatial directions of the 2D OMA image must have a dimension equal to a power of two. The images of the Hα line from the cascade arc plasma have a spectral dimension of 512 and a spatial dimension of 400. Since the spatial dimension is not a power of 2, it must be increased to a power of two greater than 400. This is accomplished by padding the spatial dimension of the image with enough zeros to form a 512 spectral by 512 spatial array (spatial rows 401 through 512 contain zeros). After padding the image array to the correct dimension, the image of the Hα line intensity is Abel inverted. The result is a 512 spectral by 256 spatial array of the radial distribution of line emission needed for determination of the radial distribution of electron number density.
5.2.4 Determination of Electron Number Density from Stark Broadening

Line emission from the hydrogen Balmer alpha, H\textsubscript{\alpha}, line results when electrons in the major quantum level \(n = 3\) of excited hydrogen atoms transition to major quantum level \(n = 2\). The discrete jump in quanta implies that this transition will result in radiation that is monochromatic \[9\]. Monochromatic emission is not the case in reality; the transition actually results in a spectral line that has a finite thickness (line broadening).

The mechanisms that lead to the broadening of a spectral line can be placed into three main categories: pressure broadening, broadening due to the Doppler effect, and Stark broadening \[9\]. Pressure broadening results from frequent collisions among radiating atoms. Pressure broadening becomes more influential as pressure increases. Line broadening due to the Doppler effect is a result of the random motion of the emitting atoms. Radiation from atoms moving away from the observation point is shifted to lower frequencies, and radiation from atoms moving toward the observation point is shifted to higher frequencies. Because higher plasma temperatures result in faster particle motion, the Doppler effect becomes more pronounced as the temperature increases. Stark broadening results when electric microfields set up by charged particles perturb the normal energy levels of the emitting atoms \[9\]. Perturbations in the energy levels lead to shifts in the frequency of the radiation and cause the line to broaden. The Stark effect is strongly dependent on the density of the charged particles and only weakly dependent on plasma temperature \[93\]. If the effects of pressure, Doppler, and Stark broadening were removed, the line would still have a finite width called the natural width. The natural width of a line is associated with uncertainty in the exact energy levels in the line.
transition, which is related to the Heisenberg uncertainty principle [78]. The natural width of a line is generally much smaller than Doppler broadening [9].

Boulos defines the plasma that results from the high intensity arcs seen in cascade arcs as thermal plasmas [9]. In thermal plasmas, natural broadening is insignificant when compared to Doppler and Stark broadening. The Doppler effect usually results in small contributions to line broadening in thermal plasmas; Stark broadening typically predominates [9]. "The Stark effect becomes predominate as soon as the rate of ionization exceeds one percent." [9]

Because the Stark effect has strong dependence on electron number densities and depends only slightly on temperature, the electron density of a plasma can be determined independently of the plasma temperature by comparing theoretical line widths to the experimentally measured Hα lines [61]. Since the measured line of sight intensities from the Hα line have been Abel inverted into a radial distribution of Hα line emissions, a radial distribution of Hα line profiles is available for use in determining the radial distribution of electron number density. This is accomplished through the comparison of experimental and theoretical Stark broadened lineshapes. Modeling Stark broadening to obtain theoretical lineshapes is not a simple task. Analytic solutions have not been obtained without simplifying assumptions or Monte Carlo computer simulations [94]. A brief discussion of the theoretical Stark broadening solutions and their implications is presented below.

5.2.4.1 Introduction to Stark Broadening

The Hα line is Stark broadened when the electric microfield of a charged particle perturbs the energy levels of an emitting atom during the emission process.
Two different time quantities are necessary to characterize this process. The first is the time for which the charged particle is perturbing the atom—the perturbation time. It is given by [9]:

$$\tau_s = \frac{b}{\bar{V}}$$  \hspace{1cm} (5.4)

where

- $b$ = the impact parameter
- $\bar{V}$ = the relative mean velocity of the charged particle with respect to the emitting atom.

The perturbation time is the time for which the charged particle is considered to be colliding with the excited atom. For a weakly coupled plasma, the Debye radius is the largest impact parameter ($b$ in equation (5.4)) of importance, and the collision time becomes [95]:

$$\tau_s = \frac{\rho_D}{\bar{V}}$$  \hspace{1cm} (5.5)

where

- $\rho_D$ = Debye radius given by [9]

$$\rho_D = \sqrt{\frac{\varepsilon_0 k T_e}{e^2 n_e}}$$  \hspace{1cm} (5.6)

and

- $\varepsilon_0$ = permittivity of free space,
- $k$ = Boltzmann's constant,
- $T_e$ = electron temperature,
\[ n_e = \text{electron number density}. \]

As inferred from equations (5.5) and (5.6), the collision (perturbation) time for a weakly coupled plasma is inversely proportional to square root of the electron number density. The second quantity of time used to characterize Stark broadening is the 'Time of Interest' (TOI) defined as the "time required for the destruction of optical coherence." [95]

Interactions, or collisions, of charged particles with the emitting atom during this TOI results in Stark broadening. The collision time and the TOI characterize Stark broadening and lead to models that make analysis of this broadening mechanism possible. The static ion model and the dynamic ion model are two models have been developed for this purpose.

5.2.4.2 Stark Broadening--the Static Ion Model

The static ion model led to the first theoretical solutions to Stark broadening [95]. This model assumes two different limiting extremes for the electron and ion perturbers in a plasma [95]. The relative velocities between the electrons and emitting atoms are assumed to be large enough to allow a complete collision to occur within the time of interest (TOI--discussed in the previous section). The electrons are at what is known as the impact limit--the collisions are complete within the time of interest \( \tau_s < \text{TOI} \). On the other hand, the relative velocities between the ions and emitting atoms are assumed to be small enough that their movement is considered insignificant during the TOI. Thus, a quasistatic approximation is made for the ions,
and their effects on the plasma are simply averaged over the static electric microfield [95].

Many solutions to Stark broadening have been obtained using the static ion model [95], the most widely used were developed by Hans Griem [93, 61]. These sources have tabulations of the theoretical profiles of Stark broadened hydrogen lines for the electron number densities and temperatures realized in thermal plasmas. Through comparison of a measured Stark broadened emission profile with the theoretical profiles in Griem's tables, the electron number density corresponding to the measured profile can be ascertained (only an estimate of the temperature is required because of Stark broadening's weak temperature dependence). Since the radial distribution of $H_\alpha$ emission profiles is known, the radial distribution of electron number densities in the cascade arc can be obtained. This is accomplished using a computer code to find the best theoretical profile for the measured experimental emission line at each of the radial locations in the Abel inverted image. The fitting program adjusts the amplitude and spectral position of the theoretical emission line, in addition to the electron number density and heavy particle temperature corresponding to the line, to find the best fit possible. The best fit profile is established by minimizing the sum of the square of the differences between the measured and theoretical profiles. Results from this analysis are presented in Chapter 6.

5.2.4.3 Stark Broadening--the Dynamic Ion Model

In the dynamic ion model, the quasistatic ion assumption is relaxed. Therefore, the effects of the ions must be simulated using Monte Carlo methods to generate time-dependent electric microfields in the plasma [94]. The effects of
electron collisions with the emitting atoms are included in these calculations [95].
The results of these Monte Carlo simulations give the half width at half maximum of
the stark broadened emission line over the range of electron number densities and
temperatures of interest in thermal plasmas. As in the static ion case, the half widths
are only weakly dependent on plasma temperature in the dynamic ion model.

A couple of interesting results from the dynamic ion modeling need to be
mentioned. Relaxing the static ion assumption results in emission profiles that are
Lorentzian. The Stark profiles obtained using the static ion model have broader
wings than those predicted by the dynamic ion model (Figure 5.7). As the quasistatic
ion limit is approached in the dynamic ion model, the line profiles are very similar to
those predicted using the static ion model [95]. The implication of the differences in
the predicted line profiles leads to drastically different electron number densities
associated with the same emission line half width. This effect is intensified for lower
electron densities. "Calculations show that at low electron densities, ion dynamics
increases the half-width of H\textsubscript{\alpha} of neutral hydrogen several fold." [94] Figure 5.8
shows the variation of the full width at half maximum (FWHM) of a Stark broadened
H\textsubscript{\alpha} line with electron number density. Three curves appear in this figure—one for
Stark broadening assuming static ion perturbers and the other two for Stark
broadening assuming dynamic ion perturbers. Notice that the static and dynamic ion
curves are starting to converge at higher electron densities, as expected. The two
dynamic ion curves represent Stark broadening for H\textsubscript{\alpha} with either helium ions or
hydrogen ions (protons) as the perturbers of the emitting hydrogen atom. Stark
broadening has been found to be sensitive to the mass of the perturbing ion [95] as
indicated by the separation of the dynamic ion curves in Figure 5.8. The width of the
Stark broadened line scales inversely with the reduced mass of the emitting
Figure 5.7 Comparison of Hα emission profiles as predicted by both the static ion model and the dynamic ion model.
Figure 5.8 Variation of the full width at half maximum of a Stark broadened H\text{\textalpha} line with electron number density.

Adapted from:
atom/perturber pair raised to the 0.4 power [95]. Therefore, broadening data with perturber B can be scaled to broadening data with perturber A of a different mass using:

\[
FWHM_A = \left( \frac{\mu_B}{\mu_A} \right)^{0.4} FWHM_B
\]  
(5.7)

where

\[
FWHM_A = \text{the full width at half maximum of the line Stark broadened by perturber A,}
\]

\[
FWHM_B = \text{the full width at half maximum of the line Stark broadened by perturber B,}
\]

\[
\mu_A = \text{reduced mass of emitting atom/perturber A pair}
\]

\[
= \frac{\text{mass}_A \cdot \text{mass}_\text{atom}}{\text{mass}_A + \text{mass}_\text{atom}}
\]

\[
\mu_B = \text{reduced mass of emitting atom/perturber B pair.}
\]

Equation (5.7) is consistent with the differences seen between the proton, and helium ion perturber curves in Figure 5.8.

Good agreement has been found between the Stark broadening results with helium ion perturbers and the experimentally measured Stark broadening of the H_\alpha line in a helium arc seeded with two percent hydrogen [94, 96]. At the writing of this dissertation, the literature contains no data with which to validate the Stark broadening of H_\alpha by protons. For the data collected from the UTSI cascade arc operating on pure hydrogen, the dynamic broadening with proton perturbers was used to analyze the electron number density. For the simulated ammonia and hydrazine
mixtures, equation (5.7) was used to scale the proton perturber data to account for the effects of nitrogen perturbers.

To obtain the radial distribution of electron number density in the cascade arc using the results from the dynamic ion model, the width of the $\text{H}_\alpha$ emission line at every radial location in the cascade arc needs to be determined. At the pressures tested, the line broadening contribution due to the Doppler effect might be significant in comparison to the Stark broadening effect. The resulting line profile would be a Voigt profile—a convolution of Gaussian (Doppler) and Lorentzian (Stark) lineshapes. A downhill simplex computer algorithm [97] was used to fit a Voigt profile to the experimental data at each radial location. In this computer algorithm, the electron number density, heavy particle temperature, spectral position of the theoretical emission line, amplitude of the theoretical emission line, and amplitude of the background noise are optimized to achieve the best fit possible. From the results of this fitting routine, line widths for both the Lorentzian and Gaussian components of the Voigt profile were determined. The Lorentzian line width (the Stark broadening component of the profile) at each radial location was then correlated with the broadening data in Figure 5.8 to obtain the electron number density at the corresponding radius. As will be seen in the next chapter, the emission profiles are essentially Lorentzian—the Gaussian component is insignificant within experiment uncertainty. As expected, the Stark broadening realized in the cascade arc plasmas is better represented by the dynamic ion theory which does not neglect the important effects of ion motion.
5.3 Determination of Electron Temperature

In general, the temperature of a plasma is of interest to the scientific community. A rough estimate of the plasma electron temperature can be made by utilizing line emission of several different excitation states of the same atom. Line emission from atomic state \( n \) to \( m \) is given by [9]:

\[
\varepsilon_{nm} = \frac{h}{4\pi} A_{nm} N_n \nu_{nm}
\]  

(5.8)

where

\( \varepsilon_{nm} \) = line emission coefficient corresponding to transition from atomic excited state \( n \) to \( m \),

\( A_{nm} \) = the transition probability from atomic state \( n \) to \( m \),

\( N_n \) = the number density of excited state \( n \),

\( \nu_{nm} \) = frequency associated with electronic transition from state \( n \) to \( m \),

\( h \) = Planck's constant.

If a Boltzmann distribution of electron populations at some electron temperature is assumed, then the electron population of atomic state \( n \) can be written [9]:

\[
\frac{N_n}{N_o} = \frac{g_n e^{-E_n/(kT_e)}}{g_o}
\]  

(5.9)

where

\( N_o \) = number density of the ground state,

\( g_n \) = degeneracy of state \( n \),

\( g_o \) = degeneracy of the ground state,

\( E_n \) = energy of atomic state \( n \),
\( T_e = \text{electron temperature}, \)
\( k = \text{Boltzmann's constant}. \)

Substitution of equation (5.9) into equation (5.8), and some algebraic manipulation yields:

\[
\ln \left[ \frac{4 \pi e_{nm} g_0}{h \lambda_{nm} \nu_{nm} g_n} \right] - \ln[N_0] = -E_n \left( \frac{1}{kT_e} \right) \tag{5.10}
\]

The unknowns in equation (5.10) are the electron temperature and the ground state number density. If the first logarithm on the left hand side of equation (5.10) is plotted against the energy of the excited state, \( E_n \), for all of the measured emissions lines, then an estimate of the electron temperature can be obtained from the slope of the best fit line through all points on the plot. The natural logarithm of the ground state number density on the left hand side of equation (5.10) does not effect the electron temperature calculation; it only vertically shifts the position of the curve. This plot is called a Boltzmann plot. The electron temperature is given by:

\[
T_e = -\frac{1}{k \cdot \text{slope}} \tag{5.11}
\]

To obtain estimates of plasma electron temperature distributions in the 50 A hydrogen arcs at 2 psi and 6 psi, emission profiles of the H\( \alpha \), H\( \beta \), H\( \gamma \), and H\( \delta \) lines were used to make radially resolved Boltzmann plots. The emission profiles were obtained using the Abel inversion technique described in Section 5.2. This data was collected in the second order to guarantee an accurate estimate of the continuum. A standard tungsten filament lamp was used to calibrate the spectral sensitivity of the
detector over the range defined by these spectral lines. A typical Boltzmann plot for a 50 A hydrogen arc at 6.0 psi is shown in Figure 5.9. Since the above analysis results in a Boltzmann plot at every radial location, an estimate of the radial distribution of electron temperature can be obtained (the results are presented in Chapter 6).

The nonequilibrium nature of the plasmas realized in the UTSI cascade arc render these electron temperature measurements quite inaccurate because the Boltzmann plot assumes that all bound and free electrons have the same temperature—a poor assumption for the cascade arc plasmas. Therefore, the electron temperatures obtained using this method are rough estimates of the real values and should only be considered indicators of trends in the true electron temperatures. Two important facts add justification to this statement. First, because of spectral dispersion limits of the spectrometer/grating combination, it was not possible to fit the H_α, H_β, H_γ, and H_δ emission lines on the OMA detector at the same time. Each line had to be measured individually. Therefore, the relative line intensities are more difficult to establish, and the uncertainty in the Boltzmann plot increases. This effect is complicated by the low intensities of the H_γ and H_δ lines. Second, the electron temperature inaccuracies are due to a characteristic of hydrogen. The transitions utilized in the calculations are for the same ionization state of the same element (atomic hydrogen). There is relatively small difference between the upper states of these transitions. This leads to small energy differences between the states that are typically not much larger than the thermal energy in the plasma [61]. "Relative line intensities from the same element and ionization stage do not result in accurate temperatures." [61] With hydrogen, this problem cannot be remedied by measuring
Figure 5.9 A Boltzmann plot using the $H_{\alpha}$, $H_{\beta}$, $H_{\gamma}$, and $H_{\delta}$ transitions in a 50 A hydrogen arc at 6.0 psi at a radius of 1.5 mm.

different emission lines from different ionization stages because the only hydrogen ion (the proton) cannot be electronically excited.
COMPARISON OF EXPERIMENTAL AND NUMERICAL RESULTS

The results of the hydrogen, simulated ammonia (NH$_3$), and simulated hydrazine (N$_2$H$_4$) cascade arc experiments are presented in this chapter. The axial electric field, the radial distribution of electron number density, and the electron temperature for the hydrogen arcs are presented first. The electron number density distributions are presented for both of the Stark broadening models described in Chapter 5. These experimental results are compared with hydrogen plasma simulation results from the Cascade Arc Plasma Simulation (CAPS) code. Experimental results for the hydrogen/nitrogen mixtures simulating ammonia and hydrazine follow the discussion of the hydrogen results. The chapter is concluded with a detailed discussion of the experimental results. All of the experimental results presented in this chapter were obtained using the data analysis procedures discussed in Chapter 5. Detailed discussions of the CAPS code and simulation results are found in Chapters 2 and 4, respectively.

6.1 Hydrogen Results

The cascade arc was operated with pure hydrogen arcs at 2.0 psi and 6.0 psi and a current of 50 A. Nine different sets of data were taken at each condition and the data were analyzed using the methods described in Chapter 5. The axial electric
field, radial distribution of electron number density, and radial distribution of electron
temperature are discussed in Subsections 6.1.1 through 6.1.3, respectively.

6.1.1 Comparison of Experimental Axial Electric Field and Power with CAPS
Code Simulation Results

Table 6.1 shows a comparison of the experimental and numerical electric field
for the 2.0 psi and 6.0 psi cases. The experimental electric fields were determined by
finding the slope of the best fit line through the measured potentials of the cascade
plates (see Chapter 5). The simulated axial electric fields are from the CAPS code
simulations using the different finite rate chemical kinetic rates discussed in Chapter 4.
The electric fields from the equilibrium simulations overpredict the experimentally
determined values by 33 percent for the 2.0 psi case and 10 percent for the 6.0 psi
case. These overpredictions increase to 180 percent and 51 percent for the 'Slow'
nonequilibrium simulations at 2.0 psi and 6.0 psi, respectively. The electric field for
the 'Fast' nonequilibrium simulations overpredicts the experiment by 17 percent for
2.0 psi and agrees with the value for 6.0 psi. The 'Fast' reflective wall nonequilibrium
case matches the electric field for 2 psi, but underpredicts the value for 6 psi by 14
percent. The 'U of I' nonequilibrium simulations best predict the electric field,
underpredicting the experimental values for the 2.0 psi case within 4 percent and
matching the values for the 6.0 psi case. It is evident that the chemical kinetic rates
have a large impact on the electric field realized in the nonequilibrium computer
simulations.
Table 6.1 Comparison of experimentally determined electric field (V/cm) with UTSI Cascade Arc Plasma Simulation (CAPS) code values.

<table>
<thead>
<tr>
<th></th>
<th>Equilibrium Simulation</th>
<th>'Slow' Non-Equilibrium</th>
<th>'Fast' Non-Equilibrium</th>
<th>'Fast' Reflective Wall</th>
<th>'U of I' Non-Equilibrium</th>
<th>Experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1: 2.0 psi</td>
<td>46.4</td>
<td>95.7</td>
<td>42.0</td>
<td>36.4</td>
<td>33.4</td>
<td>36.0 ± 1.2</td>
</tr>
<tr>
<td>Case 2: 6.0 psi</td>
<td>46.3</td>
<td>64.9</td>
<td>43.9</td>
<td>36.9</td>
<td>44.1</td>
<td>44.2 ± 1.2</td>
</tr>
</tbody>
</table>

Good agreement between the power deposited into the plasma and the power removed from the plasma is a good check for the experimentally determined axial electric field. Table 6.2 is a comparison of the electrical power deposited into the plasma with the power removed by the cooling water. Calculations of these experimental values are discussed in Chapter 5. For both 2 psi and 6 psi, the measured power removed from the plasma agrees with the electrical power deposited into the plasma within experimental uncertainty. Therefore, the experimental electric field is consistent with the measured plasma power. Comparisons of the measured plasma power with the CAPS code simulation results have the same trends as the electric field comparisons. A discussion of the CAPS code simulation results appears in Chapter 4 and will not be repeated here.
Table 6.2 Comparison of experimentally determined arc power with UTSI Cascade Arc Plasma Simulation (CAPS) code values.

<table>
<thead>
<tr>
<th></th>
<th>Power In [W/cm]</th>
<th>Power Out [W/cm]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>2.0 psi</td>
<td>6.0 psi</td>
</tr>
<tr>
<td>Experiment</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pressure</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.0 psi</td>
<td>1965. ±278.</td>
<td>1965. ±278.</td>
</tr>
<tr>
<td>2.0 psi</td>
<td>1965. ±278.</td>
<td>1965. ±278.</td>
</tr>
<tr>
<td>Pressure</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Experiment</td>
<td>1807. ±60.</td>
<td>2267.</td>
</tr>
<tr>
<td>Equilibrium</td>
<td></td>
<td></td>
</tr>
<tr>
<td>'Slow' Non-Equilibrium</td>
<td>4785.</td>
<td>3178.</td>
</tr>
<tr>
<td>'Fast' Non-Equilibrium</td>
<td>2099.</td>
<td>2179.</td>
</tr>
<tr>
<td>'U of I' Non-Equilibrium</td>
<td>1670.</td>
<td>2223.</td>
</tr>
<tr>
<td>'Fast' Reflective</td>
<td>1821.</td>
<td>1850.</td>
</tr>
</tbody>
</table>
6.1.2 Comparison of Experimental Radial Distribution of Electron Number Density with CAPS Code Simulation Results

The optimum FIR smoothing filter used in the Abel inversion algorithm for eliminating high frequency spatial noise had a cutoff frequency of 4 percent of the Nyquist frequency, and the FIR filter for removing high frequency spectral noise had a cut off frequency of 20 percent and 6 percent of Nyquist frequency for the 2 psi and 6 psi hydrogen cases, respectively. After completion of the Abel inversion, the radial profile of line emissions was available for the determination of the electron density distribution. The integrated line emission at each radial location is related to the electron number density at that radial position. A typical radial profile of the integrated emission data for the 6.0 psi case is shown in Figure 6.1. The error bars on the emission of plus or minus one standard deviation of the output noise are estimates of the error associated with the Abel inversion. This error was calculated from the variance of the input noise and the spatial bandpass cutoff frequency using a method developed by Smith [98]. Smith shows that "the variance of the output noise is directly proportional to the variance of the input noise and to the bandwidth [of the filter], and inversely proportional to the radial distance from the origin" [98]. As can be seen in Figure 6.1, the error is inversely proportional to the radius. The error asymptotically approaches infinity as the radius goes to zero. However, when the radius is as little as 20 µm, the standard deviation of the emission has decreased to a few percent of the emission and continues to decrease with radius. The emission has not decreased to zero at 2 mm, the radius of the arc constrictor. A possible explanation for this feature is that the plasma might be slightly bowed into the optical channels leading to the windows. Reflections of the high intensity arc from the walls
of the optical channel might also contribute to the non-zero intensity beyond a radius of 2 mm.

6.1.2.1 Comparison of Static Ion Stark Broadening Results with CAPS Code Simulation Results

The electron number density data presented in this section have been obtained using the static ion assumption in the Stark broadening theory. As discussed in Chapter 5, because the static ion assumption neglects the important effects of ion motion on Stark broadening, the electron number density distributions determined using the static ion Stark broadening theory are not expected to be correct. The radial distributions of 'static' electron number densities for the
hydrogen cascade arc plasmas are presented in this section to illustrate the significant error that can result with the static ion assumption. Comparisons of the radial distribution of calculated and experimental 'static' electron number densities for the 2.0 psi and 6.0 psi cases are presented in Figures 6.2 and 6.3, respectively [99]. The simulations were run using the three sets of finite chemical kinetic rates (presented in Chapter 4). The electron distributions labeled 'Ref' are simulations with 'Fast' finite rate chemical kinetics and a reflective wall model in which plasma species reflect off of the wall. The error bars on the experimental electron number densities (Figures 6.2 and 6.3) are plus or minus one standard deviation of the nine realizations at each pressure and do not directly include the error resulting from the Abel inversion. The error resulting from the Abel inversion process is not included in these error bars because this error was found to be quite small and is not believed to significantly alter the measured electron number densities (discussed in detail in Section 6.3.1.2.2). At both pressures the nonequilibrium computer simulations underpredict (as expected) the experimentally determined electron number densities for all radii and for all ionization rates by as much as 1.5 orders of magnitude.

Figure 6.4 shows a theoretical, static ion Stark broadened Hα profile fitted to 6 psi hydrogen arc data at a radius of 1.5 mm. This poor fit is typical of the those at other radii, and at the lower pressure. The overprediction of the wings leads to relatively poor fits (Figure 6.4), and amplifies the inflated number densities resulting from the incorrect static ion assumption. Because dynamic ion effects cannot be neglected, the measured emission profile is better represented by the Lorentzian profile predicted by dynamic ion Stark broadening theory (see discussion in Chapter 5). Figure 6.5 shows a Voigt profile, with a very large Lorentzian component, fitted
Figure 6.2 Comparison of experimental (static ion) and numerical radial distributions of electron number density in a 50 A hydrogen arc at 2.0 psi.
Figure 6.3 Comparison of experimental (static ion) and numerical radial distributions of electron number density in a 50 A hydrogen arc at 6.0 psi.
Figure 6.4 Measured and fitted theoretical Stark lineshapes of $H_\alpha$ line in a 50 A hydrogen arc at 6.0 psi at a radius of 1.5 mm.
Figure 6.5. Measured and fitted theoretical Voigt lineshapes of H\(_\alpha\) line in a 50 A hydrogen arc at 6.0 psi at a radius of 1.5 mm.
to the same data shown in Figure 6.4. This theoretical, dynamic ion Stark broadened H\textsubscript{\alpha} profile matches the 6.0 psi hydrogen arc data.

6.1.2.2 Comparison of Dynamic Ion Stark Broadening Results with CAPS Code Simulation Results

The static ion assumption has been relaxed for the data presented in this section--eliminating the large error that results from neglecting the significant effects of ion motion on Stark broadening. Thus, the Voigt fitting routine and dynamic ion Stark theory discussed in Chapter 5 have been implemented. The Voigt profile fit to the experimental H\textsubscript{\alpha} emission line shown in Figure 6.5 is indicative of the fits at other radii for both the 2 psi and 6 psi hydrogen cases. The Voigt profiles are predominately Lorentzian (Stark broadening) since the Gaussian profile (Doppler broadening) contribution is very small. Comparisons of the radial distribution of calculated and experimental electron number densities for the 2.0 psi and 6.0 psi cases are presented in Figures 6.6 and 6.7, respectively. The error bars on the experimental electron number densities (Figures 6.6 and 6.7) are plus or minus one standard deviation of the nine realizations at each pressure and do not directly include the error resulting from Abel inversion (discussed in detail in Section 6.3.1.2.2).

At 6.0 psi, the nonequilibrium computer simulations underpredict or match the experimentally determined electron number densities at all radii and for all ionization rates. At 2.0 psi, the experimental electron number densities are bounded by the electron number densities predicted using the nonequilibrium code. While the "dynamic" electron number densities are underpredicted by about an order of magnitude for the 'Slow' cases at both pressures, the results for the 'Fast' case reduce
Figure 6.6 Comparison of experimental (dynamic ion) and numerical radial distributions of electron number density in a 50 A hydrogen arc at 2.0 psi.
Figure 6.7 Comparison of experimental (dynamic ion) and numerical radial distributions of electron number density in a 50 A hydrogen arc at 6.0 psi.
this error significantly for small radii. The 'Fast' case matches the experiment at smaller radii at 6.0 psi and overpredicts the experiment by about a factor of two at 2.0 psi. However, for radii beyond approximately 1.2 mm, the 'Fast' case results in large underpredictions. The 'U of I' case gives the best nonequilibrium solution results; it underpredicts the 6.0 psi experimental values by less than 50 percent and overpredicts the experimental value at 2.0 psi by less than a factor of two. The shape of the 'U of I' profile also gives the best agreement with that of the experiment. The equilibrium simulation predicts that the electron number density becomes negligible at a radius of 1.5 mm, while the nonequilibrium simulations predict significant electron densities all the way to the wall. This characteristic--indicative of a nonequilibrium plasma--is also clearly seen in the data.

The slope of the experimental electron number density curves close to the wall of the arc channel at 2 mm have the tendency to be positive, especially at 6.0 psi. This feature is not believed to be real. The 6.0 psi arc is more intense and constricted than the arc at 2.0 psi. Therefore, the 6.0 psi arc has a smaller diameter. Figure 6.8 shows high speed images of the 50 A hydrogen arcs. The photos on the left side of the figure are unaltered images of the H\textsubscript{\alpha} line with the intensity reduced via neutral density (N.D.) filters to prevent camera damage. In an effort to better define the edge of the arcs, the photos on the left side of Figure 6.8 were filtered using the auto-contrast feature in photo processing software. The resulting images are shown on the right side of the figure. As seen in the pictures, the 2.0 psi arc fills the constrictor and the 6.0 psi arc has a diameter roughly equal to 3.3 mm, which corresponds approximately to the location where the slope of the electron density curve has the tendency to go positive. Images were collected over a range of frequencies to ensure that the arcs were not traveling around the constrictor; no arc motion was apparent.
Figure 6.8 High speed images of 50 A hydrogen arcs at 2.0 psi and 6.0 psi.
The positive slope in the electron number density profile close to the wall could be explained by a combination of three factors, all magnified by a low signal level at larger radii. First, plasma contaminates with low ionization potentials (e.g. copper atoms) could be present. However, no traces of non-hydrogen emission lines were seen in any spectra collected. Second, some of the light from the broader lines near the arc center can reflect off of the optical channels so that the light appears to be originating closer to the constrictor wall. This reflected light effectively broadens the thinner and weaker line emission near the walls and leads to measured electron densities larger than they are in reality. Third, it is very difficult to determine the exact magnitude of the continuum. A small increase in the background level can cause artificial line broadening during Abel inversion. A parametric study was performed to determine the sensitivity of the electron number density profile to the magnitude of the continuum. Small shifts artificially added to the magnitude of the continuum did not significantly affect the features of the electron number density profile. Therefore, the positive slope near the wall is attributed mostly to reflections (See Section 6.3 for further discussion).

6.1.3 Comparison of Experimental Radial Distribution of Electron Temperature with CAPS Code Simulation Results

The electron temperatures presented in this section are determined from Boltzmann plots. It must be stressed that the nonequilibrium nature of the UTSI cascade arc plasmas leads to large error in the resulting electron temperature (see Chapter 5 for details). Therefore, the electron temperature data presented in this section are not expected to represent the true electron temperature. However, the
data can be utilized to determine trends. Figures 6.9 and 6.10 show comparisons of the radial distributions of calculated and experimental electron temperatures for the 2.0 psi and 6.0 psi cases, respectively. Only the 'U of I' nonequilibrium solutions are presented in these plots for the sake of clarity. The computer simulations overpredict the experimental centerline temperature by approximately a factor of three for the 2.0 psi case and match the experiment (within experimental error) for the 6.0 psi case. As anticipated, the measured temperature profiles do not match any of the simulation temperature distributions. The negative temperature gradient at the constrictor wall and the large error of the experimental temperature distributions make these preliminary data very questionable. The error bars on the experimental data are plus or minus one standard deviation calculated from the uncertainty associated with the slope of the line in the Boltzmann plot (the Boltzmann plot of a 6 psi hydrogen arc is shown in Figure 5.9). The relatively large error bars in the measured electron temperature results from poor fits through the four data points in the Boltzmann plots. The uncertainty in the measured electron temperature is further increased by the fact that emission lines from higher ionization stages are not available in hydrogen and cannot be included in the Boltzmann plots. As discussed in Chapter 5, the measured temperatures are not accurate and should only be used to indicate trends.

6.2 Simulated Ammonia and Hydrazine Results

The cascade arc was also operated with simulated ammonia (NH₃) and hydrazine (N₂H₄) at 2.0 psi, 6.0 psi, and 10.0 psi at 50 A. Three different sets of data were taken at each pressure and the data were analyzed using the methods
Figure 6.9 Comparison of Experimental and Numerical Radial Distributions of the Plasma Temperature in a 50 A Hydrogen Arc at 2.0 psi. 'U of I' indicates a finite rate solution using 'U of I' kinetics.
Figure 6.10 Comparison of Experimental and Numerical Radial Distributions of the Plasma Temperature in a 50 A Hydrogen Arc at 6.0 psi. 'U of I' indicates a finite rate solution using 'U of I' kinetics.
described in Chapter 5. The axial electric field and radial distribution of electron number density are discussed in Sections 6.2.1 and 6.2.2, respectively.

6.2.1 Axial Electric Field

The axial electric fields of the hydrogen/nitrogen mixtures are determined in the same way as for pure hydrogen. Table 6.3 shows a comparison of experimentally determined electric fields for the hydrogen and hydrogen/nitrogen mixtures. For the pressure range tested, the electric field increases with pressure and decreases as nitrogen content increases.

Table 6.3 Experimental pressure variation of electric field (V/cm) for hydrogen, simulated ammonia, and simulated hydrazine.

<table>
<thead>
<tr>
<th></th>
<th>Hydrogen</th>
<th>Simulated Ammonia</th>
<th>Simulated Hydrazine</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1:</td>
<td>2.0 psi</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>36.0 ± 1.2</td>
<td>26.4 ± 0.7</td>
<td>26.2 ± 0.8</td>
</tr>
<tr>
<td>Case 2:</td>
<td>6.0 psi</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>44.2 ± 1.2</td>
<td>38.8 ± 1.1</td>
<td>35.1 ± 0.9</td>
</tr>
</tbody>
</table>
6.2.2 Radial Distribution of Electron Number Density

The spatial optimum FIR smoothing filter used in the Abel inversion algorithm had a cutoff frequency of 4 percent of the Nyquist frequency for hydrogen/nitrogen mixtures at all pressures. The spectral FIR filter had a cut off frequency of 6 percent of Nyquist frequency at 2.0 psi and 20 percent of Nyquist frequency at 6.0 psi and 10.0 psi.

The radial distribution of experimental electron number densities obtained using dynamic ion Stark broadening theory for simulated ammonia and simulated hydrazine are shown in Figures 6.11 and 6.12, respectively. The electron density increases with pressure for both mixtures. Because the nitrogen content of hydrazine

![Graph](image_url)

Figure 6.11 Radial distributions of electron number densities (dynamic ion) for simulated ammonia (NH₃) at 2.0 psi, 6.0 psi, and 10.0 psi.
(N₂H₄) is higher than it is in ammonia (NH₃), the hydrazine arc has slightly higher electron densities over the pressure range tested. An interesting feature of the profiles is the positive slope of the curve close to the wall of the arc channel at 2 mm. This feature is also seen in the hydrogen plasmas and is explained by the same phenomena.

6.3 Discussion of Results

A discussion of the results presented above and any ramifications of these results are discussed in this section. The 50 A hydrogen arc results are discussed in Section 6.3.1, and the 50 A simulated ammonia and simulated hydrazine arc results are discussed in Section 6.3.2.
6.3.1 Discussion of Hydrogen Results

This section contains a discussion of the comparison of experimental results for the 50 A hydrogen arcs at 2.0 psi and 6.0 psi with the CAPS code simulation results. Explanations for any discrepancies realized in these comparisons will be offered. The axial electric field results, the radial distributions of electron number density, and the radial distributions of electron temperature are presented in Sections 6.3.1.1 through 6.3.1.3, respectively.

6.3.1.1 Axial Electric Fields for Hydrogen

Determination of the experimental axial electric field from the easily measured potentials of cascade arc constrictor plates requires very simple analysis (see Chapter 5). Because this analysis of the measured plate potentials is a simple one-step procedure, a high degree of confidence is placed in the resulting electric fields. The self consistency of the measured power balance increases the confidence in the electric field measurement (refer to Section 6.1.1).

As presented in Table 6.1, variation of the finite rate chemical kinetics highly influences the predicted axial electric field. By varying the chemical kinetic rates, the simulated electric fields bound the measured electric fields in hydrogen plasmas. The 'U of I' chemical kinetic rate set best predicts the measured axial electric field for the 50 A hydrogen arcs at 2.0 psi and 6.0 psi. Therefore, confidence in the 'U of I' simulations is higher than any of the other simulations.
6.3.1.2 **Explanation of Discrepancies in Electron Number Density Comparisons**

The comparison of the radial distributions of electron number density presented in Section 6.1.2 show discrepancies ranging from as low as 50 percent to as high as 1.5 orders of magnitude. The magnitude of the discrepancy depends on which chemical kinetic rates were utilized in the CAPS code simulations and whether the static ion or dynamic ion assumption was utilized in the Stark broadening theory implemented in the data analysis. As expected, the results presented in Section 6.2.2 confirm that the dynamic ion assumption is necessary for the proper analysis of the hydrogen plasmas realized in the cascade arc. Not only are the discrepancies between the experimental and simulated electron number density distributions significantly reduced from the static ion results, the measured line emission profiles are Lorentzian (as predicted by dynamic ion Stark broadening theory). Unfortunately, discrepancies in electron number densities still exist between the computer simulation results and the "dynamic ion" experimental results. These discrepancies result from either error in the CAPS code simulations, experimental error, or a combination of the two. Possible sources of error in the computer simulations and the experiment are discussed in Sections 6.3.1.2.1 and 6.3.1.2.2, respectively.

6.3.1.2.1 **Discussion of Uncertainty in CAPS Code Simulations**

As established in Chapter 4, all of the CAPS code simulations are well converged. Therefore, the simulation results are internally self consistent and would not change significantly with extended iterations. Even though the simulations are well converged, other possible sources of error in the CAPS code could contribute to the discrepancies in the comparisons of the simulated and experimental electron
number densities. These include effects associated with the size of the computation grid, the boundary conditions utilized in the CAPS code, errors in the finite rate chemical kinetics, and errors in the nonequilibrium transport properties.

The sensitivity of computational fluid dynamic (CFD) simulation results on the computation grid are well established [100]. In general, the greater the grid density (more grid points in the same space), the better the CFD code models a gas flow. Unfortunately, more grid points usually result in more computations and a longer time until code convergence. Therefore, it is best to utilize a computation grid with as few grid points as possible without compromising the accuracy of the CFD solution.

Because the CAPS code is a CFD code, it is important to establish the effects of the computation grid on the simulations. The CAPS code simulation results used in the comparisons with experimental data were all performed on a computation grid with 31 radial grid locations. To determine whether this grid density is adequate, the number of radial grid points was increased to 61 (doubling the grid density). The solution of the denser grid changed less than one percent from the 31 point grid solution. Since this substantial increase in grid density had very little effect on the solution, the computation grid with 31 radial grid points is believed to be adequate.

In the CAPS code, the plasma in contact with the wall is assumed to satisfy a no slip condition, and the wall temperature is assumed to be fixed at 300 K. As stated in Chapter 4, the simulation results are quite insensitive to the value of the fixed wall temperature. Increasing the wall temperature to 900 K (the melting point of copper is 1083.4 K [101]) changed the simulated axial electric field and plasma power less than 0.3 percent and the centerline electron number density less than 5 percent. The wall boundary is also assumed to be catalytic—allowing all chemical reactions to come to completion instantaneously (see Chapter 2). These assumptions are not unrealistic for
the water cooled walls of the cascade arc constrictor. However, the experimental
data with which the computer simulation results are compared is collected through a
window into the cascade arc constrictor. An open channel connects the constrictor in
the center of the constrictor plate to the window on the plate edge. Therefore, the
constrictor wall does not define the edge of the arc where optical data is collected.
Each of four windows in the window section has an optical channel to the constrictor.
The existence of these optical channels not only introduces uncertainty into the
validity of the wall boundary conditions utilized in the simulations, it increases the
uncertainty of the one-dimensionality assumed in the problem. The entrances to these
four optical channels are only 1/16" high. Because the optical channels are a
relatively small portion of the constrictor wall, the plasma is not believed to bow
significantly into the optical channels—as verified in the experiment (see Figure 6.8).
In this case, the one-dimensional assumption is sufficient. Because the constrictor
and optical channel walls in the copper window section are water cooled and optical
channel entrances are only 1/16" high, the hydrogen gas in the optical channels is
assumed to be cool. With this assumption and the fact that the simulations are quite
insensitive to the value of the fixed wall temperature, a catalytic wall boundary
condition at 300 K is appropriate. Any deviations in this boundary condition from
reality would introduce uncertainty into the CAPS code simulation results.

A parametric study was carried out to determine the sensitivity of the CAPS
code simulation results to the finite rate chemical kinetics. This entailed changing the
finite rate chemical kinetic rate for each individual reaction in the 'U of I' reaction set
as much as two orders of magnitude and running the CAPS code to convergence.
Individually changing the kinetic rates for the first four reactions in the 'U of I'
reaction set (see Table 4.4) two orders of magnitude changed the peak electron
density less than four percent while changing the axial electric field up to 17 percent. The largest of these changes in the predicted electron densities and the predicted electric field resulted when reactions involving molecular hydrogen were altered. On the other hand, changing the rates for the recombination of atomic hydrogen (the second and fourth reaction in Table 4.4) by two orders of magnitude resulted in peak electron density and electric field changes of less than one percent. The stability of the CAPS code simulation was most sensitive to changes in the reaction defining the recombination/ionization of atomic hydrogen by electrons (reaction five in Table 4.4). Both increasing and decreasing this rate by as little as 100 percent resulted in an unstable CAPS code simulation that would not converge. Reaction rate changes of less than 50 percent resulted in approximate changes in the electron density and electric fields of percent 5 percent and 0.5 percent, respectively. In general, none of the rate changes made in this parametric study of the 'U of I' reaction rate set resulted in a substantial improvement in the simulated electron number density profile without pushing the simulated electric fields far out of agreement with the experimental values.

A parametric study was also performed to determine the effects of changes in the nonequilibrium transport properties on the computer simulation results. For reference, unaltered nonequilibrium transport properties from the CAPS code simulations (with the 'U of I' chemical kinetics shown in Table 4.4) of the 50 A hydrogen arcs near the centerline are shown in Table 6.4. Each transport property was artificially changed up to plus or minus fifty percent, and the CAPS code was run to convergence (see Table 6.5). Artificially changing the electrical conductivity had the highest impact on simulation results for both pressures. The predicted electron number densities approached the "dynamic ion" electron number densities, although
Table 6.4 Nonequilibrium transport properties from CAPS code simulations ('U of I' chemical kinetics) of 50 A hydrogen arcs at 2.0 psi and 6.0 psi near the arc center.

<table>
<thead>
<tr>
<th>Transport Property</th>
<th>Case 1: 2.0 psi</th>
<th>Case 2: 6.0 psi</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electrical Conductivity [mhos/m]</td>
<td>$2.26 \times 10^3$</td>
<td>$2.56 \times 10^3$</td>
</tr>
<tr>
<td>Kinematic Viscosity [m$^2$/sec]</td>
<td>$7.02 \times 10^{-5}$</td>
<td>$7.28 \times 10^{-5}$</td>
</tr>
<tr>
<td>Thermal Conductivity [Watts/m-K]</td>
<td>1.77</td>
<td>1.97</td>
</tr>
<tr>
<td>Diffusion Coefficient [m$^2$/sec]</td>
<td>$1.39 \times 10^{-4}$</td>
<td>$1.18 \times 10^{-4}$</td>
</tr>
</tbody>
</table>
Table 6.5 Effects of artificial variation of calculated nonequilibrium transport properties on CAPS code simulations using 'U of I' finite rate chemical kinetics.

<table>
<thead>
<tr>
<th>Transport Property</th>
<th>Artificial Change [Percent]</th>
<th>Pressure [psi]</th>
<th>Axial Electric Field [V/cm]</th>
<th>Peak Electron Number Density [1/m³]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unaltered baseline</td>
<td>0</td>
<td>6.0</td>
<td>44.1</td>
<td>1.06 x 10^{22}</td>
</tr>
<tr>
<td>Electrical conductivity</td>
<td>-50</td>
<td>6.0</td>
<td>58.1</td>
<td>1.74 x 10^{22}</td>
</tr>
<tr>
<td>Species diffusion</td>
<td>-50</td>
<td>6.0</td>
<td>38.2</td>
<td>1.59 x 10^{22}</td>
</tr>
<tr>
<td>Electron and heavy particle thermal conductivities</td>
<td>-50</td>
<td>6.0</td>
<td>37.3</td>
<td>1.19 x 10^{22}</td>
</tr>
<tr>
<td>Viscosity</td>
<td>-50</td>
<td>6.0</td>
<td>44.1</td>
<td>1.06 x 10^{22}</td>
</tr>
<tr>
<td>Unaltered baseline</td>
<td>0</td>
<td>2.0</td>
<td>33.4</td>
<td>3.59 x 10^{21}</td>
</tr>
<tr>
<td>Electrical conductivity</td>
<td>+50</td>
<td>2.0</td>
<td>27.3</td>
<td>3.07 x 10^{21}</td>
</tr>
<tr>
<td>Species diffusion</td>
<td>+50</td>
<td>2.0</td>
<td>34.6</td>
<td>3.19 x 10^{21}</td>
</tr>
<tr>
<td>Electron and heavy particle thermal conductivities</td>
<td>+50</td>
<td>2.0</td>
<td>37.9</td>
<td>3.72 x 10^{21}</td>
</tr>
<tr>
<td>Viscosity</td>
<td>+50</td>
<td>2.0</td>
<td>33.5</td>
<td>3.59 x 10^{21}</td>
</tr>
</tbody>
</table>
agreement was not obtained. In addition, this artificial change in electrical conductivity created discrepancies in the electric field comparisons. Artificially changing the other transport properties resulted in less improvement in the electron density comparisons but still created discrepancies in the electric field comparisons. It should be noted that altering the viscosity had relatively little effect on the simulation results. This low sensitivity to viscosity is attributed to the small axial gradients realized in the cascade arc. In general, for every transport property artificially altered, the discrepancy in the electric field comparisons increased when the discrepancies in the electron number density comparisons decreased. This parametric study indicates that artificial changes in the nonequilibrium transport properties cannot reduce the discrepancies in the electron number densities at both 2.0 psi and 6.0 psi without having adverse effects on the simulated axial electric fields—which are already in good agreement with experiment.

Obviously, incorrect finite rate chemical kinetics and nonequilibrium transport properties could lead to the discrepancies in the electron number density distributions. However, it seems unlikely that changes in these properties could resolve the discrepancies in the electron number densities without adversely affecting the simulated electric field which already shows good agreement for one set of chemical kinetics and transport properties (simulations with the 'U of I' rates). The computation grid has been verified not to influence the simulation results, and the boundary conditions are reasonable given the assumptions in the CAPS code. Therefore, the uncertainties associated with the CAPS code simulations are not large enough, by themselves, to explain the discrepancies between the simulated and experimental electron number densities.
6.3.1.2.2 Discussion of Uncertainty in the Experiment and Data Analysis

As discussed in Section 6.3.1.1, relatively little uncertainty (less than 3.3 percent) is associated with the experimentally determined axial electric fields which, in general, are in good agreement with the results of the 'U of I' simulations—also believed to have a low uncertainty (see Section 6.3.1.2.1). Because the simulated axial electric field strongly depends on the radial distribution of electrons (see equation (2.23)), it is reasonable to expect that the uncertainty in the simulated electron number densities is also relatively low. The same cannot be said for the experimentally determined radial distributions of electron number density. Discrepancies between the experimental "dynamic" and simulated electron densities are as large as 200 percent for the 'U of I' simulations. Since the uncertainty in the simulated electron densities is believed to be low, the majority of the discrepancies between the calculated and experimentally determined electron densities can be attributed to uncertainty in the experimental values. This uncertainty is associated with both the raw Hα emission line data and the processing of this data.

Any uncertainty associated with the raw Hα line intensity data is attributed to both the experimental setup and the data acquisition process during operation of the cascade arc. Details of the experimental setup are discussed in Chapter 3. Because great effort was made to ensure proper alignment of the cascade arc apparatus with the external optics, misalignment is an unlikely source of experimental error. The 1.25 m Spex spectrometer was also aligned and calibrated prior to data acquisition to minimize the slit function and maximize the spectral resolution. The spatial and spectral calibration of the optical system, including the 2-D OMA with image intensifier, were also performed very carefully to minimize experimental error. The attention given to the calibration of the optical setup provides the necessary data to
eliminate as much error as possible from the raw data—any remaining error results from physical limitations of the optical setup.

Several potential error sources are present during data acquisition. While operating the cascade arc, the pressure, current, and potential drop in the plasma were continually monitored to ensure steady state operation of the device. Therefore, drift in these parameters is believed to introduce little error into the data. Any impurities in the hydrogen plasma could also introduce error into the data. It is unlikely, however, that the hydrogen test gas is a source of impurities—the hydrogen used in the experiments was 99.999 percent pure. Impurities from materials inside the cascade arc could be introduced by the vaporization of materials with low ionization potentials that would lead to higher electron densities than expected with pure hydrogen. In the hydrogen spectra analyzed, however, no emission lines from impurities were found. Therefore, impurities are believed to be minimal and introduce little error into the intensity data. The greatest source of experimental error is attributed to reflections in the window section of the cascade arc. Broad emission lines from the arc center reflect off of the constrictor walls and off of the window on the back side of the constrictor making the much thinner emission lines near the edge of the arc appear larger than they really are. This effect is only noticeable in regions near the constrictor wall where line intensities are very small and leads to unrealistically large measured electron number densities. While it is very difficult to quantify the total uncertainty introduced during data acquisition, it is unlikely this uncertainty is large enough to account for the majority of the discrepancies between the experimental and simulated electron number densities.

The analysis that transforms the raw line intensity data into radial distributions of electron number density is another significant source of uncertainty. This data
analysis requires several steps (see Chapter 5). Each of these steps introduces some uncertainty into the resulting electron number density distribution. Altogether, the multi-step process leads to uncertainty in the electron number densities significantly larger than that associated with the computer simulations. The following paragraphs discuss the uncertainty associated with each step in the analysis process.

It can be difficult to determine the exact value of the background noise with a high degree of precision. Small changes in the intensity magnitude can lead to incorrect emission line shapes during Abel inversion. Therefore, small changes in the magnitude of the measured background could potentially result in incorrect emission profiles and ultimately lead to wrong electron number densities. The background noise varied as much as 3 percent for the hydrogen cascade arc runs. A parametric study was performed to determine how small magnitude shifts in the background affect the electron number density. Magnitude shifts up to 3 percent resulted in imperceptible changes in electron number density profiles. This insensitivity of the experimental electron densities to changes in the background results in little uncertainty associated with the removal of background noise from the raw intensity data.

Removal of the slit curvature from the spectral dimension of the 2-D intensity data is a straightforward procedure that introduces little error into the analysis of the optical data. The slit curvature, depicted in Figure 5.4, is very small, and only slight spectral shifts are required to spectrally align the image. The cascade arc intensity data shown in Figure 5.3 has not had the slit curvature removed. As can be seen, the slit curvature in this image is barely perceptible near the edge of the arc--necessitating only minor spectral shifts and introducing little error to the data.
The deconvolution of the slit function from the line intensity data is performed using a digital Wiener filter, equation (5.3). As stated in the detailed discussion on the slit deconvolution (Chapter 5), the Wiener filter utilizes a smoothing constant to eliminate the possibility of a division by zero error. This constant is called the smoothing constant because it has the tendency to smooth the deconvolved data. Test functions comprised of the convolution of known Gaussian profiles were run through the Wiener filter to determine the effects of the smoothing constant. The known Gaussian profiles had specified widths corresponding to the width of the unaltered $H_\alpha$ intensity line at either 2.0 psi or 6.0 psi and the width of the measured slit function. A smoothing constant equal to 0.001 was chosen for the deconvolution of the measured slit function from the cascade arc. This value was found to give the best combination of noise reduction in the intensity data without artificially broadening the lines. Therefore, low uncertainty is attributed to this step in the data analysis.

The Abel inversion algorithm used to transform the line of sight, spatially resolved line intensity data into a radial distribution of line emission has a quantifiable error associated with it. This error is calculated using a method developed by Smith [98]. As stated in Section 6.1.2, the error is inversely proportional to the radius and asymptotically approaches infinity as the radius goes to zero. For the radial distribution of Abel inverted $H_\alpha$ emission lines from the cascade arc, the error is infinite on the centerline. In general, when the radius is as little as 20 $\mu$m, the standard deviation of the emission has decreased to a few percent of the emission and continues to decrease with radius. Near the arc center, the error associated with Abel inversion introduces significant uncertainty into the line fitting process used to determine the electron number density from the emission line.
The error associated with fitting a theoretical Stark broadened profile to the emission line depends on whether the perturbing ions in the Stark broadening theory are assumed to be static or dynamic. The uncertainty associated with the static ion results (Section 6.1.2.1) is very large and will not be discussed, since the static ion model is not appropriate for cascade arc plasmas. The electron number densities determined from the dynamic ion Stark broadening theory do have considerable uncertainty associated with them. These experimental electron number densities are determined by fitting Voigt profiles to the radial distribution of Hα emission line profiles and correlating the width of the Voigt profile's Lorentzian component to the width of a theoretical, "dynamic" Stark broadened line. The nonequilibrium 'U of I' simulations better predict the experimental distributions of electron number density (dynamic ion results) than any of the other CAPS code simulations. However, the discrepancies between the 'U of I' simulation results and the experimental results are as large as 50 percent for the 6.0 psi case and 200 percent for the 2.0 psi case. The magnitude of the error accumulated in the analysis steps leading to the radial distribution of line emission profiles is not large enough to explain the discrepancies between the simulated and experimental electron densities. Any other error associated with the data analysis of the "dynamic" Stark broadening results is associated with three sources: uncertainty in the Voigt profile fitting routine; uncertainty in the theoretical values of the "dynamic" Stark broadened emission line widths; and the quality of the emission line data being analyzed. The uncertainty in the theoretical values for the "dynamic" Stark broadened emission line widths was estimated by Oza et. al. [94] to be approximately 10 percent. This error contribution is significant, but cannot account for all of the discrepancies in the electron number density comparisons.
As previously discussed, the Voigt profile fitting routine results in excellent theoretical fits to the experimental emission profiles (Figure 6.5). However, the sensitivity of the electron number densities to the fitted Voigt profiles was not known *a priori*, and needed to be investigated. By utilizing the radial distributions of heavy particle temperature and electron number density from the 'U of I' Caps code simulations, radial distributions of simulated Voigt profiles were constructed. These profiles were fitted to the experimental emission profiles to get a feel for the sensitivity of the electron densities to the fitted Voigt profiles. The results of this study are shown in Figures 6.13 through 6.16. Each of these figures contains an experimental emission line profile and three fitted Voigt profiles. (Note that the experimental profiles at small radii--Figures 6.13 and 6.15--are much noisier than the experimental profiles at larger radii--Figures 6.14 and 6.16. This is an expected result of the Abel inversion process.) The fitted Voigt profiles labeled "Sim. T, Ne profile" are simulated profiles constructed using the simulated ('U of I') temperatures (Gaussian component) and simulated electron number densities (Lorentzian component). The profiles labeled "Sim. Ne profile" are simulated Voigt profiles constructed using the electron number densities from the 'U of I' simulations to determine the Lorentzian components of the Voigt profiles; the downhill Simplex routine finds the best Gaussian (Doppler) components. As stated previously, the emission profiles are largely Lorentzian and fitted Voigt profiles are relatively insensitive to their Gaussian components. This leads to very minor differences between the profiles labeled "Sim. T, Ne profile" and the profiles labeled "Sim. Ne profile". The Voigt profiles labeled "Best fit Voigt" were obtained from the downhill simplex fitting routine to determine both the Lorentzian and Gaussian components of
Figure 6.13 Comparison of 'Best fit Voigt' profile and simulated Voigt profiles calculated from the 'U of I' simulation results for a 50 A hydrogen arc at 6.0 psi at a radius of 0.03 mm.
Figure 6.14 Comparison of 'Best fit Voigt' profile and simulated Voigt profiles calculated from the 'U of I' simulation results for a 50 A hydrogen arc at 6.0 psi at a radius of 1.5 mm.
Figure 6.15 Comparison of 'Best fit Voigt' profile and simulated Voigt profiles calculated from the 'U of I' simulation results for a 50 A hydrogen arc at 2.0 psi at a radius of 0.03 mm.
Figure 6.16 Comparison of 'Best fit Voigt' profile and simulated Voigt profiles calculated from the 'U of I' simulation results for a 50 A hydrogen arc at 2.0 psi at a radius of 1.5 mm.
the profile. These are the Voigt profiles from which the experimental electron number densities are obtained.

Figures 6.13 and 6.14 contain comparisons of the fitted Voigt profiles to the H\textsc{\textalpha} emission lines from a 50 Å hydrogen arc at 6.0 psi at radii of 0.03 mm and 1.5 mm, respectively. The emission line data at the small radius is quite noisy and leads to relatively poor fits. At the smaller radius, the simulated profiles are broader than the "Best fit Voigt" profiles. However, the simulated profiles appear to represent the noisy experimental data as well as the "Best fit Voigt" profile does. At a radius of 1.5 mm, the simulated profiles and the "Best fit Voigt" profile are virtually indistinguishable and represent the experimental results equally well. In an attempt to quantify the error associated with the "Best fit Voigt" profile and the simulated Voigt profiles, the sum of the square of the difference between the experimental emission profile and the fitted Voigt profiles over all spectral locations was determined. This calculation was repeated for every radial position. The results of this analysis are shown in Figure 6.17. Because the "Sim. T, Ne" and the "Sim. Ne" profiles are so similar, only the "Sim. Ne" case is shown in the figure. The "Best fit Voigt" profiles generally have smaller error, and the error in the simulated profile fits are greatest near the centerline where the largest discrepancies in the electron number density comparisons are realized for the 6.0 psi case. However, not only is the maximum error in the simulated profile fits less than a few percent of the total line emission, the error due to Abel inversion was not taken into account in the downhill Simplex fitting routine. The Abel inversion error is largest on centerline and would significantly reduce the error in the simulated Voigt fits near centerline. Taking this into account, the simulated Voigt profiles calculated from the 'U of I' simulation results are believed to adequately predict the experimental emission profiles. Therefore, the radial
distribution of electron number density from the 'U of I' simulation at 6.0 psi predicts the experimental electron densities much better than indicated in Figure 6.7. The large sensitivity of the electron number density to the Voigt fitting routine leads to experimental uncertainty that accounts for most of the discrepancy between the simulated and experimental electron densities at 6.0 psi.

The analysis of the sensitivity of the electron number densities to the Voigt profile fits was repeated for the 2.0 psi hydrogen arc data. Figures 6.15 and 6.16 contain comparisons of the fitted Voigt profiles to the Hγ emission lines from a 50 A hydrogen arc at 2.0 psi at radii of 0.03 mm and 1.5 mm, respectively. Only slight differences exist between the "Best fit Voigt" and simulated Voigt profiles at a radius of 0.03 mm, all of which reasonably predict the experimental emission profile (Figure
6.15). This is expected because the 'U of I' simulation correctly predicts the experimentally determined electron number densities near the centerline for the 2.0 psi case (see Figure 6.6). For radii beyond about 1.0 mm, the simulated Voigt profiles do not predict the experimental emission profiles nearly as well as the "Best fit Voigt" profiles. Figure 6.16 shows the Voigt profile fits to the measured emission line at a radius of 1.5 mm. This radius corresponds to the largest discrepancy in the electron number density comparisons for the 2.0 psi case (see Figure 6.6). Therefore, the fits of the simulated Voigt profiles at the 1.5 mm radius are worse than the fits at any other location. At this radius the simulated profiles are broader than the measured emission line indicating larger simulated electron number densities than realized in the experiment. Figure 6.18 shows the radial distribution of the error in the simulated and "Best fit Voigt" profiles for the 2.0 psi case. As was seen for the 6.0 psi case, the "Best fit Voigt" profiles generally have smaller error; but, unlike the 6.0 psi case, the error in the simulated profile fits at 2.0 psi are greatest near a radius of 1.5 mm where the largest discrepancy in the electron number density comparison is realized. The largest Voigt fitting error is, however, less than a few percent of the line emission at that same radius. The results of the above analysis indicates that, even though the sensitivity of the electron number density to the Voigt fitting routine is quite significant, this sensitivity cannot account for all of the discrepancies in the electron number density comparisons for the 2.0 psi case as it did for the 6.0 psi case.

In addition to the sensitivity of the electron number densities to the Voigt fitting routine, the quality of the experimental emission profiles affects the uncertainty associated with the experimentally determined electron number densities. The cascade arc emission line data is potentially degraded by three sources: self absorption of the H\textalpha line, high frequency noise, and low intensity signal.
Figure 6.18  Radial distribution of error associated with the 'Best fit Voigt' profile and simulated Voigt profiles calculated from the 'U of I' simulation results at 2.0 psi.

Any self absorption of the $H_\alpha$ line would lower the peak of the emission line and effectively broaden the line shape. A characteristic feature of a self absorbed line is a dip in the emission at the spectral center of the line. None of the $H_\alpha$ line data collected had this feature; therefore, the line is not strongly self absorbed. However, weaker self absorption will tend to flatten the peak of the emission line, instead of creating a dip. This situation will also broaden the line, although to a lesser degree. To determine the extent of self absorption of the $H_\alpha$ line in the cascade arc data, the optical thickness, $\tau_\nu$, of the plasma was calculated. The optical thickness of a plasma is given by [9]:

$$\tau_\nu = \kappa_\nu' L$$

(6.1)

where
\( \kappa'_v = \text{the absorption coefficient at wavelength } v, \)
\( L = \text{the characteristic length of the plasma}. \)

The absorption coefficient of the \( H_\alpha \) line is calculated using the methods given in Boulos [9]. If the plasma is optically thick \((\tau_v >> 1)\), self absorption is significant. If the plasma is optically thin \((\tau_v << 1)\), line emission passes through the plasma without being absorbed. The optical thickness for the \( H_\alpha \) line in the 6.0 psi hydrogen arc was calculated to be approximately 0.01. Therefore, this hydrogen plasma is relatively thin for the \( H_\alpha \) line, and self absorption should be fairly insignificant. This same result was obtained by other researchers for a hydrogen plasma, under similar conditions but generated in a different device, where self absorption was both calculated and experimentally demonstrated to be insignificant [102]. Because plasmas are more optically thick at higher pressures, the 2.0 psi hydrogen plasma in the cascade arc is also optically thin. Therefore, self absorption is not believed to significantly degrade the \( H_\alpha \) line emission data.

The same is not true for the effects of high frequency noise and low signal in the \( H_\alpha \) line emission data. The high frequency noise is filtered during Abel inversion, and the associated error was discussed previously. The low intensity signal results in small signal to background noise ratios across the entire arc. The spectrally resolved signal to noise ratios of the unaltered intensity data of the \( H_\alpha \) line at radii near the centerline and approximately 1.5 mm are shown in Figures 6.19 and 6.20 for the 6.0 psi and 2.0 psi cases, respectively. The maximum signal to noise ratios occur near the center of the arc and have values less than 2.4 for both pressures. As the edge of the arc is approached, the signal decreases significantly. This is also true as one moves spectrally away from the spectral center of the \( H_\alpha \) line. Therefore, the intensity signal
Figure 6.19 Spectrally resolved signal to background noise ratios of the $H\alpha$ line intensities near centerline and at a radius of 1.5 mm for a 50 A hydrogen arc at 6.0 psi.
Figure 6.20  Spectrally resolved signal to background noise ratios of the H\textsubscript{\alpha} line intensities near centerline and at a radius of 1.5 mm for a 50 A hydrogen arc at 2.0 psi.
in the wings is quite poor. This effect is more profound for the 2.0 psi arc at larger radii. Because of long exposure times used in the data acquisition and the physical limitations of the 2-D OMA/image intensifier combination, significantly larger signal to noise ratios were unobtainable. The low signal of the $H_\alpha$ line intensity amplifies the uncertainty in the Voigt line fitting discussed above.

As seen in Figures 6.19 and 6.20, the width of the $H_\alpha$ line is much smaller at 2.0 psi than at 6.0 psi. In the Abel inversion routine, the emission lines are transformed into the Fourier domain. After being transformed, the thinner lines at 2.0 psi are comprised of higher frequencies than the wider lines at 6.0 psi. The highest frequency components add definition to the lineshape—especially in the wings. Unfortunately, the experimental emission data has high frequency noise that interferes with the details of the lineshape. To some degree, the high frequency noise and the high frequency components of the line become indistinguishable. The high frequency noise has to be filtered out for the fitting routines to work properly. This results in the removal of detail in the lineshape—removing definition from the wing and effectively narrowing the line. Though this effect is relatively insignificant for the broad lines realized at 6.0 psi, it has great impact on the much narrower lines at 2.0 psi, especially at larger radii where the intensity is very low. Figure 6.21 shows a comparison of the signal to noise ratio of the spectral $H_\alpha$ line profiles for the 2.0 psi and 6.0 psi cases at a radius of about 1.5 mm. This plot emphasizes the narrowness of the 2.0 psi lineshape and the low intensity in the wings.

The error associated with the experimental data and the data analysis introduces a lot of uncertainty into the radial distributions of electron number density. Most of this uncertainty is attributed to three sources: the sensitivity of the electron densities to the Voigt fitting routine; the 10 percent uncertainty associated with the
6.3.1.3 Discussion of Electron Temperature Distribution Comparisons

As previously explained, the measured electron temperatures in the hydrogen arcs have large error associated with them and are not expected to represent the actual electron temperature (see Sections 5.3 and 6.1.3 for details). However, they
can be considered indicators of trends in the electron temperatures. With this in mind, it can be observed that the electron temperatures are highest on centerline, as expected. This trend is also seen in the 'U of I' simulation results; however, the simulations predict significantly higher electron temperatures. The very large uncertainty associated with the measured electron temperatures at 2.0 psi and 6.0 psi (Figures 6.9 and 6.10) make it impossible to determine which pressure has the higher electron temperature—the 'U of I' simulations predict a higher centerline electron temperature for the 2.0 psi case.

The measured electron temperature profiles have the tendency to tail up near the wall, just like the electron number density profiles. It is believed that this feature in the electron temperature distribution is false and results when emission from hotter lines near the center of the arc reflects off of the optical channel walls in a way that makes it appear to originate from the region of weaker line emission near the constrictor wall (especially for the H$_7$ and H$_8$ emission lines). These reflections corrupt the true line emissions and lead to electron temperatures that appear hotter near the wall than they are in reality.

6.3.2 Discussion of Simulated Ammonia and Hydrazine Results

Two observations were made as a result of the cascade arc experiments using simulated ammonia and simulated hydrazine. First, the electron number densities increased with pressure over the range of pressures tested. Second, the electron densities increased as the percentage of nitrogen increased. Because the axial electric field is inversely proportional to the concentration of electrons, the trends in the electric field oppose the trends in the electron densities. In general, the axial electric
field is inversely proportional to the nitrogen concentration and proportional to the pressure. Because a hydrogen/nitrogen CAPS code is beyond the scope of this dissertation, simulation results of the ammonia and hydrazine cascade arc are not available for comparison with experimental results.
CHAPTER 7

CONCLUSIONS AND RECOMMENDATIONS

Radial distributions of electron number density and axial electric fields were experimentally determined for the UTSI cascade arc operating on pure hydrogen, simulated ammonia (NH₃), and simulated hydrazine (N₂H₄). Details of the experiment, data analysis, and results were presented in Chapters 3, 5, and 6, respectively. The measured hydrogen plasma conditions have been compared to results from the Cascade Arc Plasma Simulation (CAPS) code for several different sets of finite rate chemical kinetics (see Chapter 6). Details of the CAPS code and simulation results were discussed in Chapters 2 and 4, respectively. This chapter presents conclusions drawn from the work detailed in previous chapters and makes recommendations for future work.

7.1 Conclusions

Nonequilibrium plasma conditions of 50 A hydrogen arcs at 2.0 psi and 6.0 psi have been measured. The radial distributions of electron number density and the axial electric fields were determined from the measured data, and the results were compared with UTSI CAPS code simulation results.

The experimental electron number densities were obtained by fitting theoretical emission lines predicted by Stark broadening theory to the experimentally determined radial distributions of the H₅ emission line. The experimentally
determined electron densities realized in the experiment depend on the assumed effects of ion motion. For the static ion assumption, the important effects of ion motion on Stark broadening are neglected. Therefore, the electron number densities determined from this theory are not expected to be correct. This expectation was confirmed using H\textsubscript{\alpha} emission line data from the UTSI cascade arc. Because dynamic ion effects cannot be neglected, the measured emission profiles are better represented by the Lorentzian profiles predicted by dynamic ion Stark broadening theory. These Lorentzian lineshapes result in lowered electron number densities that are better predicted by the CAPS code simulations.

Simulations of the 2.0 psi and 6.0 psi hydrogen arcs have been run with a wide range of chemical kinetics. The simulated plasma conditions were found to be extremely sensitive to the kinetics. By varying the chemical kinetic rates, the simulated electric fields bound the measured electric fields in hydrogen plasmas. The CAPS code simulations utilizing the 'U of I' chemical kinetic rate set predict the measured axial electric field for the 50 A hydrogen arcs at both 2.0 psi and 6.0 psi. The 'U of I' simulations also gives the best predictions of the experimental electron number densities; it underpredicts the 6.0 psi experimental electron number densities (dynamic ion results) by less than 50 percent and overpredicts the experimental values at 2.0 psi by less than a factor of two. The shape of the 'U of I' profile also gives the best agreement with that of the experiment.

The uncertainty associated with the experimentally determined electron number densities is believed to account for the discrepancies between the experimental electron densities and those from the 'U of I' simulation. This uncertainty is attributed to three sources: the sensitivity of the electron densities to the Voigt fitting routine; the uncertainty in the theory that correlates theoretical dynamic
ion Stark broadened line widths to electron number densities; and the low intensity signal from the H$_\alpha$ emission line. Although it has not been quantified, the total uncertainty in the measured electron number densities makes it very difficult to claim that the electron densities predicted by the 'U of I' simulations are wrong. The 'U of I' chemical kinetic rate set, therefore, is believed to be the best finite rate chemical kinetics set investigated for hydrogen in this work.

It is important to note that the 'U of I' chemical reaction set is identical to the 'Fast' chemical reaction set. The reaction rate for the dissociation of molecular hydrogen by electrons is the only difference between the 'U of I' kinetic rate set and the 'Fast' kinetic rate set. All of the other chemical reactions have identical chemical kinetic rates. Yet, the 'U of I' simulations predict experimentally determined axial electric fields and electron number density distributions substantially better than the 'Fast' simulations. The 'U of I' kinetic rate for this reaction is substantially lower [88] than the 'Fast' kinetic rate [85]. Therefore, the 'U of I' chemical kinetic rate set results in more molecular hydrogen predicted across the radius of the arc. In fact, the 'U of I' simulations have considerably more molecular hydrogen than all of the other nonequilibrium simulations (see Chapter 4), none of which predicted the experimental results better than the 'U of I' rates. This implies that a higher fraction of molecular hydrogen in the simulation results is necessary to properly predict the hydrogen cascade arc plasma. To verify this implication, the radial distribution of molecular hydrogen density is needed. These values cannot be ascertained from the spectral data collected, but can be determined through Raman spectroscopy. The acquisition of this data and comparison with simulation results is left for future work.
It should be noted that the equilibrium CAPS code simulations predict negligible electron number densities beyond a radius of 1.5 mm, while the nonequilibrium simulations predict significant electron densities all the way to the wall. Significant electron densities all the way to the wall—indicative of a nonequilibrium plasma—is also clearly seen in the data. Thus, the nonequilibrium state of the cascade arc plasma is confirmed.

Electron number density profiles for simulated ammonia and simulated hydrazine have been obtained for 50 A arcs at 2.0 psi, 6.0 psi, and 10.0 psi. The measured electric field was found to vary directly with pressure and inversely with nitrogen content. The measured electron number density followed opposite trends.

7.2 Recommendations for Future Work

Parametric studies were carried out to determine the sensitivity of the CAPS code simulation results to the finite rate chemical kinetics and the nonequilibrium transport properties. None of the changes in chemical kinetic rates resulted in substantial improvement in the simulated electron number density profiles without pushing the simulated electric fields far out of agreement with the experimental values. Similarly, none of the artificial changes in the nonequilibrium transport properties reduced the discrepancies in the electron density comparisons without creating error in the axial electric field comparisons. These parametric studies indicate that it is unlikely that either changes in the chemical kinetics or artificial changes in the nonequilibrium transport properties will lead to a reduction in the electron number density discrepancies for hydrogen at both 2.0 psi and 6.0 psi without having adverse affects on the axial electric field comparisons—which are
already in good agreement. However, the energy dependent collision cross-sections and particle interaction models utilized in the CAPS code transport property routines were not individually varied to determine their effects on simulation results. Therefore, a detailed investigation addressing the collision models in the transport property routines is merited—this investigation is left for future work.

At the writing of this dissertation, a hydrogen/nitrogen mixture version of the UTSI CAPS code was under development. Once completed, this code will allow detailed comparisons of simulation results with the electron densities and axial electric fields determined from the simulated ammonia and simulated hydrazine cascade arc experiments. These comparisons will allow the finite rate chemical kinetic and nonequilibrium transport property models for hydrogen/nitrogen mixtures to be evaluated. This study is beyond the scope of this dissertation and is left for future work.
LIST OF REFERENCES
LIST OF REFERENCES


84. Electronic Measurements Inc. brochure, "EMHP Series Three Phase AC Input SCR-Type DC Power Supplies," EMHP-REV. 5 11/93 5M.


APPENDIX A

DRAWINGS OF CASCADE ARC COMPONENTS

This appendix contains detailed engineering drawings of the UTSI Cascade Arc components that were made in-house at The University of Tennessee Space Institute. These major components include: the constrictor plates, the window section, the insulator gaskets, the cathode, the anode, the cathode housing, and the anode housing. A complete discussion of these components can be found in Chapter 3.

A.1 The Constrictor Plate

The constrictor plate is comprised of the constrictor plate, a constrictor plate cap, and two nipples that allow hookup to water cooling lines. Drawings for these components are shown in Figures A1 through A4. The cooling water nipples and plate cap are silver brazed to the constrictor plate during fabrication.

A.2 The Window Section

The window section is comprised of two modified constrictor plates, two constrictor plate caps, and four nipples that allow hookup to water cooling lines. The constrictor plate cap and the nipples are the same as those used in a regular constrictor plate. Drawings of the modified constrictor plate are shown in
Figure A1. Top view of the oxygen free high conductivity (OFHC) copper constrictor plate.
Figure A2. Side view of the OFHC copper constrictor plate.
Figure A3. Top and side views of a OFHC copper constrictor plate cap.
Figure A4. Drawing of brass or stainless steel constrictor plate nipple.
Figures A5 and A6. Fabrication of the window section starts with silver brazing the cooling water nipples and a constrictor plate cap to each of the modified constrictor plates. Then, the two halves of the window section are carefully soft soldered together to ensure that all of the optical channels line up perfectly. To aid in the alignment, a 1/8" diameter steel pin positioned in the location of the bolt hole (before the bolt holes were drilled) in each corner of the modified constrictor plate were utilized to hold the plates together during soldering. Once soldered together, these alignment pins were drilled out to form the larger diameter bolt holes. To complete fabrication of the window section, a 5 mm diameter, 1 mm thick sapphire window was epoxied into each of the four optical channels.

Figure A5. Top view of one half of the window section's modified constrictor plate.
SECTION A-A
All dimensions are inches.
Dimensions are preslider.

Figure A6. Side view of one half of the window section’s modified constrictor plate.

A.3 The Insulator Gaskets

Two kinds of insulator gaskets are utilized in the cascade arc. The first kind is a square, mica gasket with four retaining bolt holes and a central hole. This outer insulator gasket not only serves as an electrical insulator, it also forms part of the o-ring groove’s outer edge. The second kind of insulator gasket is a binderless alumina and silica paper washer. The outer edge of this insulator gasket serves as the inner edge of the o-ring groove. The gasket’s inner edge is exposed to the plasma during operation of the cascade arc. A top view of the insulator gaskets is shown in Figure A7. Both gaskets are 1/32" thick.
Figure A7. Top view of the inner and outer insulator gaskets.
A.4 The Anode

In addition to the two pieces of thin walled steel tubing (one with 0.250" OD and 0.030" wall thickness, the other with 0.125" OD and 0.020" wall thickness), the anode is comprised of a 2% thoriated tungsten anode tip, the top and bottom components of the OFHC copper anode tip holder, and an OFHC copper washer. Drawings of the latter four are shown in Figures A8 through A11, respectively. The anode tip is silver brazed to the top component of the anode tip holder. All other joints are soft soldered. Refer to Chapter 3 for a description of the anode assembly.

A.5 The Cathode

The cathode is made from a 2% thoriated tungsten cathode tip silver soldered to a piece of 1/4" stainless steel tubing. A drawing of the cathode tip is shown in Figure A12.

![Tungsten Anode Tip](image)

Figure A8. Drawing of the 2% thoriated tungsten anode.

Tungsten Anode Tip
All dimensions are inches.
Fillets have 0.030" radius.
Figure A9. Drawing of the top component of the OFHC copper anode tip holder.
Copper Anode Disk Holder (Bottom)
All dimensions are inches.
All fillets have 0.030" radius.
SECTION A-A

Figure A10. Drawing of the bottom component of the OFHC copper anode tip holder.
Copper Anode Washer
All dimensions are inches. Fillets have 0.030" radius unless noted otherwise.

Figure A11. Drawing of the OFHC copper anode washer.
Figure A12. Drawing of the 2% thoriated tungsten cathode tip.
A.6 The Anode Housing

The anode housing is comprised of an OFHC copper anode housing (Figures A13 and A14), a G10 spacer (Figures A15 and A16), an OFHC copper anode housing cap (Figures A17 and A18), a constrictor plate cap, and two nipples. The nipples and constrictor plate cap are the same as those used in the constrictor plates. Fabrication involved silver brazing the constrictor cap and two nipples to the copper anode housing. 1/8" copper tubing was soft soldered into the two holes in the sides of the anode housing. This copper tubing is the passage by which test gas is removed from the cascade arc. The anode housing cap is soft soldered to the 1/4" stainless steel tubing portion of the anode.

Figure A13. Top view of the OFHC copper anode housing.
Figure A14. Side view of the OFHC copper anode housing.

Figure A15. Top view of the G10 anode spacer.
Figure A16. Side view of the G10 anode spacer.
Figure A17. Top view of the OFHC copper anode housing cap.
Figure A18. Side view of the OFHC copper anode housing cap.

A.7 The Cathode Housing

The cathode housing is comprised of an OFHC copper cathode housing (Figures A19 and A20), a boron nitride insulator (Figures A21 and A22), a G10 spacer (Figures A23 and A24), a constrictor plate cap, and five nipples. The constrictor plate cap and nipples are the same as those used in the constrictor plates. Fabrication involved silver brazing the constrictor plate cap and nipples to the copper cathode housing. Two of the nipples are brazed to the cooling water inlet and outlet; the other three are brazed to the walls of the cathode housing and act as hookups for the test gas supply lines.
Figure A19. Top view of the OFHC copper cathode housing.
Figure A20. Side view of the OFHC copper cathode housing.
Figure A21. Top view of the boron nitride cathode insulator.

Figure A22. Side view of the boron nitride cathode insulator.
Aluminum Spacing Ring
All dimensions are inches.

Figure A23. Top view of the G10 cathode spacer.
Figure A24. Side view of the G10 cathode spacer.
Operation of the cascade arc facility is complicated because several subsystems must function properly for steady state operation of the arc. A list of the steps necessary to start, operate, and turn off the cascade arc follows.

Start up procedure

1. Open regulator valves on the K bottle(s).
2. Set gas flow rate using the flow controller(s).
3. Start mechanical vacuum pump.
4. Adjust the throttle valve to obtain the desired gas pressure in the cascade constrictor.
5. Open the water supply lines.
6. Start cooling water pump.
7. Adjust the throttle valve on the cooling water subsystem to obtain the desired flow rate and water pressure in the cooling channels.
8. Turn on the direct current power supply and set the desired current.
9. Light the arc using a Tesla coil.
10. Wait for arc conditions to equilibrate (pressure, voltage, and current stop changing).
11. Adjust the pressure until the desired pressure is attained.
Data acquisition

12. Record the operating parameters and arc conditions.
13. Take image of background noise while emission from arc plasma is blocked.
14. Take images of the hydrogen Balmier alpha line or other spectrum of interest.
15. Record potential of each plate with respect to ground so that electric field can be determined.

Arc shut-down

15. Turn off the arc power supply.
16. Turn off gas flow using flow controllers.
17. Turn off mechanical pump.
18. Close the K bottle valve(s).
19. Turn off cooling water pump.
20. Turn off water supply lines.
VITA

Trevor Michael Moeller was born in Cincinnati, OH on October 25, 1968 and spent his childhood in southeastern Indiana. He graduated valedictorian of the Batesville High School class of 1987. The following August he entered Rose-Hulman Institute of Technology and received a Bachelor of Science degree in Mechanical Engineering, May 1991. During the spring of 1991, he was awarded a National Defense Science and Engineering Graduate Fellowship through the Department of Defense and entered the University of Tennessee Space Institute the next fall. In August, 1993 he received a Master of Science degree in Mechanical Engineering. He remained at UTSI to pursue his Ph.D. in Mechanical Engineering. In May 1997, he married Ms. Laurie E. Schneider. His Ph.D. was conferred the next May.