Chapter 2

Design and Numerical Modeling of Arc Heater for HF/DF Laser

2.1 Introduction

Electric arc technology finds applications in various industrial scenarios such as plasma cutting and welding, waste treatment, and low & high voltage circuit breakers for the electric power industry [85, 86]. Apart from these industrial applications electric arcs find application in an important area of development of gas lasers. These gas lasers are scalable to high power levels, which have potential applications in industrial as well as defense sector. The gas lasers in which electric arc technology has been successfully utilized are the gas dynamic lasers in general and HF/DF lasers in particular. HF/DF lasers, wavelength of 2.6- 3.4 μm, lie in the class of high power chemical lasers based on vibrational transitions. The possibility of these lasers to be scaled up to high power levels offers a great potential of employing them in various defense and industrial scenarios. However, one of their limitations is the toxicity of its constituent elements. Though HF/DF lasers can be operated based on combustion of fluorine and hydrogen as mentioned earlier in chapter 1, however, these types of lasers are difficult to use in a normal laboratory environment because of storing problems associated with fluorine etc. Further, production of lasing species through combustion poses a safety concern. In order to overcome these drawbacks and to run the chemical laser in the laboratory, an arc-driven HF laser is an excellent alternative approach. Fluorine atoms are created by dissociation of SF₆, injected directly into the arc heater with Helium and oxygen as diluents. The use of SF₆ as fluorine atoms generator avoid the danger connected with the handling of molecular fluorine.
Arc plasma heater or generator is a versatile tool for optimizing lasers parameters [24, 87] such as gas flow rate, pressure, temperature and Mach no. etc. In order to optimize processes and to control the effect generated in arc plasma, it is essential to understand the basic arc discharge phenomena[48, 88]. Numerous researchers in the field of lasers have used arc heaters as a laboratory tool for development of various laser systems such as Gas Dynamic Laser (GDL) and Hydrogen Fluoride/Deuterium Fluoride (HF/DF) chemical lasers [6, 30, 89]. The development of advanced computational techniques has enabled better modeling of physical phenomenon inside arc plasma heaters [46, 61, 64]. The variations of parameters such as temperature field, heat fluxes produced along with the variation in velocity field and material properties may be characterized for various operation conditions.

Design aspects, modeling and validation of suitable arc heater geometry for carrying out parametric studies on a kW level HF/DF laser is being taken up in this chapter. The overall mechanics of arc discharge phenomena on the basis of numerical modeling employing commercial code COMSOL is attempted for the chosen arc heater geometry. The equations for 2D axi-symmetric, weakly compressible, laminar flow with heat transfer and coupled hydrodynamic and electromagnetic equations are solved using the SIMPLE algorithm. The variations in the material properties, temperature, and velocity due to the generated arc are studied.

2.2 Design Philosophy

The design and development of kW level arc-driven HF/DF laser system is the main focus of this work. For development of a kW level HF/DF laser, a total mass flow rate of 7-8 g/s of gas mixture (Nitrogen, Sulfur Hexafluoride and Oxygen etc) is desirable
from the first principle of chemical reaction. And from the enthalpy value in the available
literature[75] for the Nitrogen at 4000K (4.68 MJ/ kg) and considering the efficiencies of
40-50% of non-transferred arc plasma torches [68], it is evident that 50 kW dc arc input
power is required to create arc plasma in mass flow rate up to 5 g/s. Therefore, a 50 kW
arc plasma heater is capable of providing 5-7 g/s of gas mixture flow rate at desired
temperature and pressure for a kW level chemical laser. For designing 50 kW arc heater
for a kW level chemical laser application, following basic requirements are considered:
i) The design and selection of electrodes (cathode and anode) for minimum erosion (to
attain pure chemical composition of lasing gas mixture)
ii) Rotation of the arc for distribution of anode heat load and thereby reducing the anode
erosion
iii) Uniform heating of large volume of gases (5-7 g/s) at temperatures of about 2000K.
iv) The stable arc operation for 10-20 seconds

2.2.1 50 kW Arc Heater Configuration

In spite of the apparent diversity of the many types of plasma generation systems
developed, nearly all of these devices have two features in common:
a) Approximate rotational symmetry about a central axis.
b) Co-axial electrodes separated by an angular gap across which the arc current passes,
and through which the gas flows.

The topology provided by these features guarantees that at least part of the gas
passing through the unit will flow through the current carrying region (arc column) where
the heating occurs.
The three principal types of configuration, which received widespread uses in plasma generation for re-entry simulation and space propulsion and other applications during 1960s [49] are:

i) Cylindrical configuration.

ii) Toroidal configuration.

iii) Constricted configuration.

The toroidal and constricted configurations have certain limitations in terms of design of the devices. In toroidal configuration, the electrodes are two water cooled copper rings. The Arc column which strikes across the angular gap separating the rings is forced to revolve about the axis of the unit by application of an external magnetic field. The absence of magnetic field results in immediate electrode burnout. Moreover, the mechanical design of device requires considerable ingenuity on the part of the designer to minimize the total area of cooled metal surface exposed to hot gases. Whereas, in constricted configuration the flow in the region of arc column is accelerated by forming the chamber as converging duct and thus causing column confinement. In addition to certain important effects upon arc behavior including increase of column voltage gradient, current density and arc temperature, the column confinement also tends to suppress column motion, a significant source of electrical and aerodynamic fluctuations. Although, constricted configuration has advantage like producing high enthalpy for applications in reentry studies and aerodynamic testing, however, the arc stability is a severe problem in this configuration. So both these configurations are undesirable for our requirement of heating gases to moderate temperatures for lasing application.

The most versatile and also in use till date for design of plasma torches is the
cylindrical configuration, which is consisting of refractory cathode (carbon or tungsten) central cathode and a surrounding water-cooled metal anode. However, the cylindrical configuration of plasma torches is to be modified for chemical laser application to cater heating of the large volume of gases. Motion of the arc column and of its terminal upon the electrode surfaces (electrode spots) is an important factor affecting electrode life and the contamination level of the emergent heated gas. In cylindrical configuration plasma generators, self-induced or natural motion of the arc column and the electrode spots is adequate to prevent anode burn out at relatively low pressure and arc input powers. However, for operation at high power and pressure levels, anode spot motion can be increased by aerodynamic means (e.g. vertex flow within the arc chamber) or by application of a magnetic field with a component normal to the current flow. In this proposed cylindrical configuration design, both the techniques i.e. aerodynamic and magnetic field are to be employed for arc stabilization.

2.2.2 Design parameters of 50 kW Arc Heater

The performance of arc plasma generators/ arc heaters using electric arcs is determined by design of the electrodes. While cathode design is the dominant factor in determining the limitations in arc operating current & power levels as well as life before maintenance, the anode design dominates the functional performance for most arc heaters, i.e. the heat & momentum transferred.

For chemical laser application the concentric cylindrical type electrode configuration (with free arc design) consisting of a thoriated tungsten water-cooled central cathode and a surrounding water-cooled OFHC (Oxygen Free High Conductivity) copper anode is suitably selected. The electrodes (anode and cathode) arrangement is
shown in fig. 2.1.

Fig.2.1: Arrangement of Electrodes for 50 kW Arc Heater

The significance of electron source in an electric arc is evident that nearly all of the total arc current results from the electron flow, and for this reason the influence of cathode material on arc performance is of primary importance. The choice of material for non-consumable electrode arc must be a compromise between the highest possible melting and boiling temperatures and the lowest possible work function. As an operational necessity such materials as tungsten, graphite, and carbon have the highest common choices by virtue of their high temperature qualities. The alkaline earth metals have much lower work functions with thorium about midway between at 3.88 eV. This is the reason why thorium is often used as alloying agent with tungsten to improve electron emission. Hence, thoriated tungsten was chosen as the cathode material taking into the account of contamination levels of graphite and carbon. Cathode diameter is decided on
the power rating of the arc heater. If arc current is less than 400A, diameter of 10-15 mm is taken. If current is 400-1000A diameter of 20-25 mm is taken.

For chemical laser application, thoriated tungsten with 2% thorium, cathode of 23 mm is chosen due to low work function, high current carrying capacity, high melting point and low contamination level.

Anode material is of OHFC copper and it has a diameter 2-2.5 times of cathode diameter, thickness of anode is calculated by the following relation depending upon the mechanical strength, cooling water pressure, chamber pressure and temperature.

Thickness of anode wall, \[ t = \frac{pr}{SE-0.6p} \]

(Allowable stress \( S = 400 \) bar at 2000 C, Joint strength \( E = 1 \), Pressure \( p = 15 \) bar)

Thickness in mm = \[ 15 \times 25.4 / (400 - 0.6 \times 15) = 0.975 \]

Taking Factor of safety as 3, \[ t = 0.975 \times 3 \text{ mm} = 2.9 \text{ or } 3 \text{ mm} \]

Boron Nitride and Alumina are suitably employed as high temperature insulators between cathode and anode. The nitrogen/argon gas is to be injected into chamber through the insulator wall with a tangential velocity establishing a swirling vortex motion. The arc gas will then pass upward around the cathode & out through anode convergent nozzle after stabilizing the arc. As the gas passes through the arc region it will be partly ionized and will emerge as high-energy plasma.

2.3 Mathematical Modeling of Arc Plasma Devices

Although electric arcs have been known for more than 200 years, many arc phenomena remain unexplained and are still open for investigation. In spite of the plenty of information on electric arcs in the literature, many observations and their interpretations are still contradictory. The retrograde motion of the cathode attachment in a transverse magnetic field is a typical example. It seems that the arc is capable of
producing a vast variety of different phenomena induced by minor changes of the arc parameters, which are frequently difficult to control. Small impurities of the electrode surfaces or of the working fluid, or minor changes of the mechanical properties of the electrodes or of their geometry may give rise to substantial changes in the behavior and appearance of the arc. This situation imposes an extremely difficult task on the theoretical description of arcs, which is still far from complete.

During this long history of commercial applications in arc plasmas, progress is often based on trial & error approach. Due to their complexity and number of possible parameter combinations, the development process relies on the practical experience of the individual developer but not directly on the existing physical knowledge about arc discharges. Since there are many unsolved problems, it is not surprising that there is still a strong and continuing interest in arc physics and technology. Present research trends are primarily directed towards a better understanding of the interaction of arcs with flow and/or magnetic fields, and the interaction with walls or electrodes. High temperature transport properties and deviations from LTE are other areas, which are of great concern.

In principle, the behavior of any arc column may be determined by solving the conservation equations with appropriate boundary conditions, provided that the thermodynamic state of the plasma and the transport coefficients are known. Even if the assumption of LTE throughout the arc column can be justified, specification of realistic boundary conditions imposes a serious problem, in addition to the mathematical difficulties of solving a system of coupled nonlinear differential equations. It is customary in such situations to introduce simplifications, which facilitate solutions of the governing equations. Although such solutions cannot describe the actual behavior of the
arc column, they frequently reveal important physical trends. Comparisons of analytical solutions with pertinent experiments may then serve as a basis for an improvement of the initial model. By “iterating” between analytical solutions and experimental results, more realistic models may be established, leading finally to the desired agreement between analysis and experiment [76].

The first attempts to solve the conservation equations for an arc column were reported by Elenbaas and Heller in 1935. Elenbaas and Heller considered an arc column in an asymptotic equilibrium flow regime, which leads to a decoupling of the energy equation from the momentum equation. As far as the energy equation is concerned this situation is identical with the case of no flow. Neglecting radiation from the arc entirely, the energy balance may be written as

\[ \text{div} \, \vec{W} - \sigma E^2 = 0 \]  
(2.1)

where

\[ W = -k \, \text{grad} \, T \]  
(2.2)

W is the heat flow vector, k the thermal conductivity, \( \sigma \) the electrical conductivity, and \( E \) the electrical field strength. According to this equation the heat source term \( \sigma E^2 \) is balanced by heat conduction i.e., heat transfer by thermal diffusion effects is also neglected. For a rotationally symmetric arc column equation 2.1 transforms (in cylindrical coordinates \( r, \phi, z \)) into equation 2.3

\[ \frac{1}{r} \frac{d}{dr} \left( r k \frac{dT}{dr} \right) + \sigma E_z^2 = 0 \]  
(2.3)

which is known as the Elenbaas-Heller equation. \( E_z \) represents the field strength in the axial direction. By introducing the heat flux potential

\[ S = \int_{r_0}^r k \, dT \]  
(2.4)
Equation 2.3 reduces to equation 2.5
\[
\frac{1}{r} \frac{d}{dr} \left( r \frac{ds}{dr} \right) + \sigma E^2_z = 0 \quad (2.5)
\]
Where S may be considered as a function of \( \sigma \). Conservation of current in the arc column may be expressed by Ohm’s law by equation 2.6.
\[
I = 2\pi E_z \int_0^R \sigma r \, dr \quad (2.6)
\]
where R represents the arc periphery.

In spite of the severe simplifications of the Elenbass-Heller model, solutions of equations 2.5 and 2.6 are still complex because of the strong non-linearity of the transport coefficients k and \( \sigma \). In order to facilitate closed form solutions, various approximations for \( S(\sigma) \) have been proposed, ranging from linear to high order polynomial approximations, and corresponding solutions of equations 2.5 and 2.6 have been reported which indicate some of the basic trends in arc column. An extension of the Elenbaas-Heller model to include radiation losses results in the following energy balance equation
\[
\frac{1}{r} \frac{d}{dr} \left( r \frac{ds}{dr} \right) + \sigma E^2_z - P_r = 0 \quad (2.7)
\]
where \( P_r \) represents radiative energy losses per unit volume and unit time. It is assumed in this model that the arc column is optically thin, i.e., there is no appreciable re-absorption of radiation within the arc column. Attempts were also made to approximate the radiation source term in equation 2.7 for facilitating closed form solutions of this equation combined with equation 2.6.

For an accurate assessment of the behavior and properties of an arc column exact values of the transport coefficients must be introduced which necessitates numerical solutions of equations 2.6 and 2.7. Although arcs with little or no superimposed gas flow...
are frequently used in the laboratory, arcs exposed to substantial flows are of great practical interest as for example in the development of arc heaters. The wall-stabilized cascaded arc with superimposed laminar flow, received particular attention because it offers the opportunity to apply scaling laws.

A simple, single-fluid description applies for modeling of the arc if the arc plasma may be assumed to be in LTE. For this situation the conservation equations expressed in cylindrical coordinates may be written as:

**Mass:**

\[
\frac{\partial}{\partial z} (\rho u) + \frac{1}{r} \frac{\partial}{\partial r} (r \rho v) = 0 \tag{2.8}
\]

**Momentum:**

\[
\rho \left( u \frac{\partial u}{\partial z} + v \frac{\partial u}{\partial r} \right) = -\frac{\partial p}{\partial z} + \frac{1}{r} \frac{\partial}{\partial r} \left( r \mu \frac{\partial u}{\partial r} \right) \tag{2.9}
\]

**Energy:**

\[
\rho \left( u \frac{\partial h}{\partial z} + v \frac{\partial h}{\partial r} \right) = \frac{1}{r} \frac{\partial}{\partial r} \left( r k \frac{\partial h}{\partial r} \right) + \sigma E_z^2 - P_r \tag{2.10}
\]

\[
\text{Current} I = 2\pi E_z \int_0^R \sigma r \, dr \tag{2.11}
\]

The mass density of the plasma is expressed by \( \rho \); \( u \) and \( v \) are the velocity components in axial (\( z \)) and radial (\( r \)) direction, respectively; \( p \) is the pressure; \( E_z \) the axial field strength; \( h \), \( \mu \), \( k \), \( c_p \), \( \sigma \), and \( P_r \) are the plasma enthalpy, viscosity, thermal conductivity, specific heat at constant pressure, electrical conductivity, and radiative energy emitted per unit volume and unit time, respectively. Equation 2.11 implies that the radial component of the current is negligible. The plasma is treated as a perfect gas so that
\[ h - h_o = \int_{r_o}^T c_p \, dT \quad (2.12) \]

\[ p = \sum_{r} n_r \, kT \quad (2.13) \]

where \( k \) represents the Boltzmann constant and \( n \), the particle densities (electrons, ions, neutrals).

In addition to the previously stated assumptions, viscous dissipation in the plasma is neglected as well as self-magnetic field effects. The flow is assumed to be steady and axially symmetric without swirl components, and re-absorption of radiation within the arc is neglected. For establishing momentum equation 2.9 and energy equation 2.10, the usual hydrodynamic and thermal boundary layer approximations have been introduced. For solving the conservation equations the temperature dependence of thermodynamic and transport properties must be known.

Because of severe gradients of the temperature and the associated particle densities in an arc, diffusion effects play an important role. As discussed previously, energy transport due to chemical reactions in the plasma (for example, dissociation and ionization) may be the dominating contribution to the total energy transfer in certain temperature intervals. These contributions, however, are included in the thermal conductivity, which, in general, becomes a strongly nonlinear function of the temperature.

Analytical solutions of the conservation equations for the entrance region have been reported by Stine and Watson[90]. In their original arc model, radiation has been entirely neglected among other simplifications. Although the results of this analysis are only qualitative without accurate predictions of local property variations, they provide
valuable guidelines for general trends. During the sixties many attempts were made to
remove some of the simplifications in the Stine-Watson model in order to improve the
still lacking agreement between experiment and theory. Unfortunately, these attempts
had only limited success because the previously mentioned strong variations of
thermodynamic and transport properties do not lend themselves to simple modeling.
Accurate predictions can only be expected from numerical solutions of the unaltered
system of conservation equations. Such solutions have been reported by Watson and
Pegot[91] for the entrance as well as for the asymptotic region and by Bower and
Incropera[92] for the asymptotic region of arcs in laminar flow.

The crucial test for the validity of these predictions is, of course, a comparison
with pertinent experiments. Taking into account the uncertainties involved in the
determination of the transport properties, the agreement between theory and experiment
is reasonable as long as the assumption of LTE holds.

As previously mentioned, the existence of LTE in an arc is more of an exception
rather than the rule. For those types of arcs, which are of primary interest in this survey,
deviations from kinetic equilibrium ($T_e>T_g$) and deviations from chemical equilibrium
(charged particle concentrations) are of importance. Possible deviations from excitation
equilibrium involving lower lying energy levels (PLTE) are less significant, although,
they may play an important role for plasma diagnostics. If, for example, $T_e>T_g$, modeling
of the arc requires adoption of a two-fluid system, which introduces additional equations
to the set of conservation equations. As the applications of plasma devices have
increased manifold in last two decades, the subject has generated a lot of interest with
numerous researchers investigating the complexities of arc phenomena[57,69-71,79].
2.4 Numerical Modeling of 50 kW Arc Heater for HF/DF Chemical Lasers

As arc modeling generally consists of solving the conservation equations of mass, energy, momentum and current, for the column and also for the arc electrodes, so these four equations determine the principal arc quantities of temperature, pressure, plasma velocity and electric potential for any given arc current. The material functions of arc plasma, the electrodes, thermal electrical conductivity, viscosity, density, and specific heat, need to be incorporated as function of temperature. With availability of modern high-speed computers, developed numerical methods and the careful use of resources, this level of detailed computation is quite feasible. Nevertheless, approximations need to be made for treatment of electrode sheath regions. However, for currents of 100A or more, detailed treatment of these regions may be omitted.

In this section the mathematical model of 50 kW non-transferred arc heater for chemical laser application is attempted. Arc heater or arc plasma generator is device in which electrical energy is converted into thermal energy of a gas by creating an electrical discharge in the flowing gas. Arc plasma is compressible fluid as well as electrical conductor so that its behavior on electric and magnetic field material boundaries is strongly influenced by fluid dynamics in addition to electro-magnetic phenomenon. There are two possibilities of creating an arc i.e. either rotating the arc with external magnetic field or free burning arc not subjected to external magnetic or convective forces which should present a natural axis of symmetry. A 2-D model is enough for the description of free burning arc. Where as 3-D model is required to study the effect of external magnetic field on an electric arc.
2.4.1 Basic Assumption

In order to model the arc Plasma the following assumptions are made:

a. The arc plasma is a Newtonian fluid and flow is laminar.

b. The arc column is supposed to be in local thermal equilibrium.

c. The exciting energy state is populated by Boltzman distribution.

d. Temperature is less the a few electron volt (1 ev = 11604 K).

e. Arc is stabilized by its own magnetic field and by external gas flow.

f. The system is in steady state.

g. Gravity effects are negligible.

h. The arc is axially symmetric, which implies that the 2D equations could be written in cylindrical coordinates.

2.4.2 Governing Equations

The mathematical modeling of an electric arc needs a multi-physics approach including fluid mechanics, thermal transfer and magneto-electrodynamics. The transport phenomena in arc heater are mainly concerned with the prediction of temperature, concentration and fluid velocity of the gas mixture. In order to model the problems mathematically, it is required to set up a series of governing equations and appropriate boundary conditions, which describe the physical phenomena in arc chamber. The basic algorithm for solving coupled fluid flow and heat transport problems by finite volume method is perfectly described by Chun-Pyo Hong and Patankar[93, 94]. The solution of 2D plasma equations as well as the heat transport inside the electrodes directly follows the Patankar approach. The system of equations is given as:
The stationary conservation equations written in generalized form as given by Patankar[94] are stated as in equation 2.14,

$$\nabla \cdot (\rho \vec{v} \Phi) = \nabla \cdot (\Gamma_\Phi \nabla \Phi) + S_\Phi \tag{2.14}$$

Where \( \rho \) is the fluid mass density, \( \vec{v} \) is the velocity vector, \( \Gamma_\Phi \) is the diffusion coefficient, \( S_\Phi \) is the source term and \( \Phi \) represents the scalar variable that must be solved in various conservation equations (2.8-2.11). \( \Phi \) can be \( T \), the temperature; \( u, v \), a component of the velocity; \( X_i \), the vapor mass fraction; or \( V \), the electric potential.

Hence, the various parameters for the fluid conservation equations along with electromagnetic and mass fraction equations may be expressed as given in 2.15 - 2.24. The source term \( S_\Phi \) in the energy equation represents Joule’s effect, the radiation losses (U), the electronic enthalpic flux and diffusion due to mass fraction gradients in gas mixtures. The losses attributed to radiation are modeled as \( 4\pi \varepsilon \sigma_N \). The calculation method for the radiative heat flux from the arc plasma to anode and cathode surfaces is studied and followed similar to that suggested by Zhu P et al and Chen X et al [67, 95]. The material radiative flux is given by black body radiation relation as \( \Phi_{RM} = \varepsilon \sigma_{SH} T^4 \), where \( \varepsilon \) = Surface emissivity and \( \sigma_{SH} \) = Stefan Boltzmann constant (5.67 x 10^{-8} W m^{-2} K^{-4}).

\( \mu, \kappa, C_p \) and \( \sigma \) are dynamic viscosity, thermal conductivity, specific heat and electrical conductivity of the gas. ‘D’ is the diffusion coefficient of the metal vapor in to the plasma gas. Since the arc plasma device has been designed primarily for laser application which considers minimum erosion of electrodes, thus, the corresponding term in equation 2.20 is shown in the most generalized form for the sake of completion. However, in the present case its effect has not been taken into account owing to the consideration of minimum electrode erosion.
Conservation equations  \( \Phi \quad \Gamma_\Phi \quad S_\Phi \)

Continuity  
\[ \frac{\partial}{\partial t} + \frac{\partial}{\partial r} \left( r \frac{\partial u}{\partial r} \right) + \frac{\partial}{\partial z} \left( \frac{\partial u}{\partial z} \right) = 0 \]  

Axial momentum  \( u \)
\[ \mu \left( \frac{\partial^2}{\partial z^2} + \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial u}{\partial r} \right) + \frac{\partial}{\partial z} \left( \frac{\partial u}{\partial z} \right) \right) + j_y B_y (2.16) \]

Radial Momentum  \( v \)
\[ \mu \left( \frac{\partial^2}{\partial z^2} + \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial v}{\partial r} \right) + \frac{\partial}{\partial z} \left( \frac{\partial v}{\partial z} \right) \right) - \mu \frac{2v}{r^2} \]  

Energy equation  \( T \)
\[ \frac{j_x^2 + j_y^2}{\sigma} - U + \frac{k_B}{2} \left( j_z \frac{\partial T}{\partial z} + j_r \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left( \frac{\rho D}{\rho C_r} \right) \frac{\partial X_i}{\partial z} \]  

Potential equation  \( V \)
\[ \sigma \]

Mass fraction equation  \( X_i \)
\[ \rho D \]

The current density components appearing in equation 2.18 are determined from the gradients of electric potential given by equations 2.21 and 2.22 respectively. The system of equations is further closed by computing the azimuthal magnetic induction \( (B_\phi) \) appearing in momentum equations 2.16 and 2.17 from the resolution of potential vector.
equations. This requires determination of two additional scalars quantities the radial ($A_r$) and axial ($A_z$) potential vector components. The terms for these scalars are determined employing equations 2.21 and 2.22 substituted in the generalized conservation equation given in equation 2.14.

Axial current density component

$$j_z = -\sigma \frac{\partial v}{\partial z}$$  \hspace{1cm} (2.21)

Radial current density component

$$j_r = -\sigma \frac{\partial v}{\partial r}$$  \hspace{1cm} (2.22)

Axial vector potential

$$A_z = \mu_0 j_z$$  \hspace{1cm} (2.23)

Radial vector potential

$$A_r = \mu_0 j_r - \frac{A_z}{\sigma}$$  \hspace{1cm} (2.24)

The azimuthal magnetic induction is then deduced as:

$$\vec{B} = \vec{\nabla} \times \vec{A}$$  \hspace{1cm} (2.25)

$$B_\theta = \frac{\partial A_r}{\partial z} - \frac{\partial A_z}{\partial r}$$  \hspace{1cm} (2.26)

2.4.3 Use of Commercial Software

There are two possible ways of treating arc plasma modeling problem: developing our own model ‘home codes’ or using commercial software. ‘Home codes’ have been used widely in the last 15 years to study specific points of arc physics, to make parametric studies or to evaluate the influence of one parameter on a simplified geometry. But current computer capability makes it possible to take into account the real geometry of a process using 3D models. Before studying the ‘arc plasma problem’, one should create the geometry (domain and grid), then developing all hydrodynamic parts in 3D and implementing electromagnetic modules to represent the presence of arc. The
hydrodynamic and electromagnetic parts are to be validated. Therefore, a very complex interface is to be developed to analyze the results, which is not a trivial task. The other possibility is the use of commercial software. These programs are sufficiently well developed and validated to describe hydrodynamic flows, and so it is possible to theoretically implement many equations or specifics of the problem. Initially, these programs were developed for description of fluid mechanics and combustion problems, so they are not particularly suited for thermal plasma processes, which characteristically have high temperatures and present large variations in transport coefficients and physical properties. A step by step validation is thus necessary to verify the developments as the source code is a black box. Nevertheless, because of the hydrodynamic developments and the possibilities for the additional modules and interfaces that make it easy to exploit the results, many commercial software packages are used by thermal plasma community: PHOENICS, FLUENT, FLOW3D, ESTET and COMSOL etc. [46].

The COMSOL Multiphysics software is based on partial differential equations (PDEs) – the fundamental equations that describe the law of science. In COMSOL, these coupled PDEs are transformed into a form suitable for numerical analysis and are solved using finite element method with high-performance solvers. With advanced solver techniques and multi-core parallel solvers, COMSOL Multiphysics optimizes computationally intensive routines for maximum performance with respect to solution times and memory consumption. The mathematical modeling of an electric arc also needs a multi-physics approach including fluid mechanics, thermal transfer and magneto electrodynamics. The corresponding conservation equations are highly coupled, on the one hand implicitly, because all thermodynamic properties and transport coefficients
depend strongly on the temperature, and on the other hand, explicitly, mainly because the flow depends on electromagnetic forces, temperature depends on Joule effects and electric field is linked to the shape and value of the temperature field [96].

Module used in COMSOL:

- Weakly Compressible Navier-Stokes (Heat Transfer Module)
- General Heat Transfer (Heat Transfer Module)
- Meridional Electric and Induction Currents, Potentials (AC/DC Module)

For the modeling of 50 kW arc heater, the COMSOL software Version 4.1 was utilized. The numerical system for arc plasma is composed of governing Navier – Stokes equations coupled with electromagnetic ones. In order to study the energy transfer between the plasma and the anode, we choose free burning arc geometry. The calculation domain of diameter 42 mm and length 100 mm is represented by a grid of cells corresponding to the \( r \times z \) directions. This grid is refined on the axis of the discharge and near the plasma–material interface. The geometry includes a tungsten cathode with a 60° angle tip. The interaction between the plasma and the cathode is not modeled. The anode studied has a radius of 21 mm. The inter-electrode distance is about 10 mm. The current intensity varies between 100 and 200 A, and the medium is at atmospheric pressure.

2.4.4 Computational Domain and Boundary Conditions

The flow field geometry of the arc plasma tunnel solved in COMSOL, version 4.1 is shown in fig.2.2. The numerical system for arc plasma is composed of governing Navier – Stokes equations coupled with electromagnetic ones. In the present studies asymmetrical configuration with a two dimensional coordination system \((r, z)\) is used in transient state. The computational domain is a simplified version of the arc heater.

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configuration selected for HF/DF laser work, but it contains all essential elements of arc operation.

A 2-D, axi-symmetric, weakly compressible, laminar flow formulation with heat transfer and induction currents/voltages has been employed. The continuity and momentum equations are solved using compressible form of SIMPLE algorithm, while the other equations use the actual computed velocity and density values. A quadrilateral mesh [fig. 2.3] has been used in the flow domain as it satisfies the conservation equations in a better manner. The anode and cathode surface are no slip wall boundaries. The gas flow inlet is primarily a velocity inlet with specified velocity of 2.5 ms⁻¹ and an argon gas density of 0.01 kg/m³ and the outlet is an open boundary. The axis is a slip boundary as the gradients normal to axis are zero.

Fig. 2.2: Field Flow Geometry of 50 kW Arc Heater

Fig. 2.3: Quadrilateral Mesh for 50 kW Arc Heater Geometry
The heat fluxes/temperatures fields are specified along the anode and cathode wall boundaries taking into consideration the interaction of these boundaries with the electric arc. The temperature boundary conditions used on the electrode surfaces are, 1000K on the anode surface (Oxygen free high conductivity copper) and 3000K on the cathode surface (thoriated tungsten). These values are considered on account of corresponding expected anode and cathode temperatures under forced water-cooling conditions and lie within the permissible limits of material melting points. The study of current-voltage characteristics of an atmospheric pressure arc shows the gas becomes ionized and conductive with rapid drop of voltage for current 100A or more and it also depicts the arc plasma torch suitable for laser application [97]. For our modeling work, the normal electric current intensity of 100A is imposed on cathode surface based on the reported values in the literature [98] and for comparison of our modeling results. While facing the cathode tip, the anode surface is assumed to be at constant potential (ground conditions) and thermal insulation condition is applied for heat transfer. As a potential boundary condition at cathode tip, we use the current density distribution \( i_z (r) = j_{\text{max}} \exp (-br) \), where \( j_{\text{max}} \) & \( b \) are constants [51]. \( j_{\text{max}} \) is commonly taken as \( 1.4 \times 10^8 \) Am\(^{-2}\) and \( b \) is calculated from \( l = 2\pi \int_0^{R_c} j(r)rdr \), \( R_c \) is the conduction radius of the arc.

The specific thermodynamic properties (mass density, specific heat), transport coefficients (thermal and electrical conductivity, viscosity), radiative losses and refractive index of argon/nitrogen are all temperature dependent and are previously calculated or taken from the literature.
2.4.5 Modeling Results

In this section modeling results achieved with Argon and Nitrogen buffers are discussed. The modeling results show that temp and velocity filed inside 50 kW arc heater with significant 2D features. The study of current/voltage characteristics of an atmospheric pressure arc shows that gas becomes ionized and conductive with a rapid drop of voltage for current of 100 Ampere or more. So for modeling of arc a normal electric current with intensity of 100 Ampere is imposed on the cathode surface based on the value reported in and for comparison with the results of their work.

2.4.5.1 Results with Argon

The foremost estimation prior to computation of domain parameters is determining the variation of material properties. Fig. 2.4 shows the variation of thermal conductivity (in Wm⁻¹K⁻¹) as function of temperature (K) for the case of argon buffer gas. It is apparent that the thermal conductivity shows a steady increase with temperature up to 15000K. This is because as temperature increases, the particle density of Argon atoms decreases monotonically due to progressive ionization, which is completed at about 15000K. Further, at higher temperatures, the density of Ar⁺ (first ionization of Argon) decreases steadily with appearance of Ar++ (second ionization of Argon), while the electron density remains almost constant. The total particle density decreases with temperature for a given pressure. At still higher temperatures, the density of Ar+++ (third ionization of Argon) starts to rise again from temperature 20000K. The ionization phenomena make a large contribution to energy transport, and corresponding thermal conductivity has a high value at the temperatures where these phenomena occur. The total thermal conductivity is considered to be the sum of the contributions from thermal
conductivities due to reactional, internal energy and translational (electrons & heavy particles) components. No ionization occurs for Argon at low temperature (T<10000K), where the translational contribution of neutral species is the most significant. But at temperature higher than 10000K, the translational thermal conductivity of electrons becomes significant. Moreover, the reactional contribution along with the contribution of the electrons also becomes important at 10000K as argon is significantly ionized. At very high temperatures, when the first ionization is completed, the translational thermal conductivity of the electrons is mainly responsible for the energy transfer until second ionization occurs [14].

![Graph showing Variation in Thermal Conductivity with change in Temperature](image)

**Fig.2.4: Variation in Thermal Conductivity with change in Temperature**

The variation in electrical conductivity (ohm^{-1} m^{-1}) along the axis for the case of argon diluent gas is shown in fig. 2.5. The electrical conductivity is found to increase with increase in temperature to a certain point beyond which it becomes nearly asymptotic to a certain maxima, which in the present case is $1.1 \times 10^4$ ohm^{-1} m^{-1}. 
Similarly, the variation of viscosity of argon with temperature is shown below in fig. 2.6. Above 10,000K, when ionization is pertinent, viscosity decreases with increasing temperatures. This drop in viscosity is due to ionization of argon, resulting in coulomb forces of relatively long range between particles.

Fig 2.5: Variation in Electrical Conductivity with change in Temperature

Fig. 2.6: Variation in Viscosity with change in Temperature
The variation of temperature along the arc length for argon plasma is shown in fig. 2.7. It is evident that the maximum temperature is reached in the zone of core of the arc plasma and the temperature decreases in both 'r' and 'z' direction as we move away from the core. The peak temperature predicted in the core is $1.51 \times 10^6$ K. However, the average flow temperature towards the exit is of the order of $1.0 \times 10^4$ K.

![Graph showing temperature variation along arc length](image)

**Fig.2.7: Variation of temperature along the arc length for argon plasma**

The planar variation of temperature contours is also shown in fig. 2.8.

![Image of temperature contours](image)

**Fig.2.8: Temperature contours of argon gas plasma**

Also, the heat flux contours corresponding to the temperatures generated in the argon gas plasma are shown in fig. 2.9. The patterns closely correspond to the region of temperature...
contours shown in the fig. 2.7&2.8 with heat fluxes being higher in the region of higher temperature except towards the exit. Heat flux is found to be high even in the region close to the exit of the arc chamber where temperatures are slightly lower than the peak temperatures.

![Heat flux contours of argon gas plasma](image)

**Fig.2.9: Heat flux contours of argon gas plasma**

Fig. 2.10 shows the variation of axial velocity along the arc length in argon gas. The planar evolution of velocity contours with a superimposed streamline plot in the

![Variation of axial velocity along argon plasma column](image)

**Fig.2.10: Variation of axial velocity along argon plasma column**
plasma column is also shown in fig. 2.11. The maximum velocities are predicted to be nearly 150 ms\(^{-1}\). The core velocities are higher with the velocities decreasing close to the wall due to viscous effects.

**Fig.2.11: Axial velocity contours of argon plasma column**

Another critical parameter that varies along the arc length is the electric potential. Fig. 2.12 shows the variation along the plasma column in case of argon diluent. It is evident that argon being easily ionizable the electric potential drops along the arc length as the ionization increases. The maximum predicted electric potential is close to 30 V.

**Fig.2.12: Variation in electric potential along the arc length**
2.4.5.2 Results with Nitrogen

Similar simulations have been carried out for plasma generation in case of nitrogen gas employing the same model. The results have been found to be qualitatively similar with minor variations owing to change in properties of buffer gas employed.

Fig. 2.13 shows the thermal conductivity variation with temperature for nitrogen gas. In the case of molecular gases like nitrogen, the thermal conductivity is a complicated function of temperature. Besides possible contributions to thermal conductivity by molecules, atoms and ions, there is substantial contribution due to chemical reactions. The peak in thermal conductivity in nitrogen compared to argon shifts to lower temperature as nitrogen dissociates to N+N at 5000 K.

Fig.2.13: Variation of Thermal conductivity with temperature for nitrogen gas

Likewise fig. 2.14 and fig. 2.15 below are depiction of variation in electrical conductivity and viscosity with increase in temperatures respectively for nitrogen buffer gas.
Fig. 2.14: Variation of electrical conductivity with temperature for nitrogen gas

Fig. 2.15: Variation of Viscosity with temperature for nitrogen gas

The variation of temperature and velocity along the arc length for nitrogen plasma are shown in fig. 2.16 & fig. 2.17 respectively. It is evident that the maximum temperature is
reached in the zone of core of the arc plasma and the temperature decreases in both ‘r’ and ‘z’ direction as we move away from the core. The maximum velocities are predicted to be nearly 90 ms\(^{-1}\) for nitrogen plasma. The core velocities are higher with the velocities decreasing close to the wall due to viscous effects.

![Graph of temperature variation along arc length in nitrogen plasma](image)

**Fig. 2.16:** Variation of temperature along the arc length in nitrogen plasma

![Graph of electric potential variation along arc length in nitrogen plasma](image)

**Fig. 2.17:** Variation of velocity along the arc length in nitrogen plasma
2.4.6 Design Validation

The experimental parametric analysis for the developed arc plasma tunnel is highly time intensive where the final aim is to employ it for laser applications. Hence, the simulation results obtained have been validated by comparing the results of axial velocity and temperature plots for argon gas given by Favalli et al. [98].

Fig. 2.18 shows the comparative variation of axial velocity along the domain with similar modeling studies performed by Favalli et al. It is evident that the results are qualitatively similar, however, the peak of axial velocities are at slightly different locations but the peak values are of nearly the same magnitude of approximately 160 ms$^{-1}$. The fall of axial velocity is more gradual in our case, which may be attributed lower current values input at the cathode coupled with different locations of minimum area of cross sections and different electrode gap.

![Axial Velocity vs Arc Length](image)

**Fig. 2.18:** Comparative plots of axial velocity variation (Magenta): Favalli et al; (Blue): Our result
Fig. 2.19 shows the comparative variation of static temperature along the domain with similar modeling studies performed by Favalli et al. It is evident that the two results are qualitatively similar, but the peak of temperature is different locations but of nearly the same magnitude. The variation as earlier can be explained on account of different locations of minimum area of cross sections and different electrode gap. The peak temperature for the reference case is 14900 K whereas for the present study the peak temperatures obtained is 14700 K.

Both results shown in fig.2.18 and fig. 2.19 are sufficient to prove that the methodology employed provides reasonable results in agreement with the ones reported in literature. Hence, the other reported results in terms of variation in material properties, heat fluxes, electric potential for both the case of argon and nitrogen plasmas are also expected to be correct. Since the geometry of each designed plasma arc tunnel is governed by specific application considerations and once the applicable computational modeled has been validated it can be employed for optimizing the parameters of the tunnel suitable for the application.
2.5 Conclusion

In this chapter numerical modeling of arc discharge using commercially available code COMSOL-Version4.1 has been attempted. The interaction between arc plasma and electrodes was studied and the profiles of variation in material properties, temperature and velocity along with heat fluxes were plotted. The results have been successfully validated with corresponding results in literature showing identical qualitative trends. The quantitative variation is attributed to the different geometry being employed specific to intended laser application. Since each arc plasma tunnel being unique the model validation paves the way for adjusting the arc parameters for achieving optimal laser operation. The experimental results of effect of variation of arc parameters on laser performance are reported in chapter 5.