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NUMERICAL MODELLING OF AN RF PLASMA TORCH WITH SWIRL

M.Z. LUO, J.S. MCFEATERS and G.D. MALLINSON

Department of Mechanical Engineering
University of Auckland
Private Bag 92019, Auckland, NEW ZEALAND

ABSTRACT

A numerical model was developed to model the behavior of the radio frequency plasma torch at Auckland University. The model incorporated a quasi-three dimensional flow field, a one dimensional electromagnetic field and accurate representation of property variations over the large temperature range. The model was solved using the PHOENICS CFD package with external routines supplied to model electromagnetic heat source terms and property variations. The results show good qualitative agreement with the experimental torch and are useful for optimizing torch design to obtain more complete particle vaporization.

NOTATION

C_p	constant pressure specific heat
E_θ	electric field intensity
F_r	radial electromagnetic body force
H_z	magnetic field intensity
h	enthalpy
I	coil current
k	thermal conductivity of the plasma gas
k_c	thermal conductivity of quartz
L_1	distance, torch inlet to beginning of coil
L_2	distance, torch inlet to end of coil
L_T	total length of torch containment tube
N	number of coil turns
p	pressure
P	electromagnetic source intensity
Pr	Prandtl number
Q	gas volume flow rate
r	radius from torch centerline
T	temperature
v_r	radial gas velocity component
v_z	axial gas velocity component
z	axial position
ρ	density
μ	viscosity
ξ	magnetic permeability of free space
ω	oscillator angular frequency
χ	phase angle
σ	electrical conductivity

INTRODUCTION

Plasma processing using radio frequency, RF, plasma torches is finding applications as a tool for materials processing. The high temperatures found in these systems allow materials to be processed in a unique environment dominated by rapid gas phase reactions. Current research at Auckland University is focused on the synthesis of titanium based ceramics such as titanium carbide, TiC, and titanium nitride, TiN, from titania, TiO_2, using an RF plasma torch.

RF plasma torches typically operate in the range of 1 to 15 MHz with power levels from 1 to 100 kW. The plasma torch at Auckland University is 15 kW and 13.52 MHz. The torch is comprised of a 42 mm ID, air cooled quartz tube surrounded by a four turn RF coil, (Figure 1 and Table I). The bulk of the gas flow through the torch is an inert gas (argon) and the reactants are added either in the gaseous form (methane or ammonia to supply sources of carbon or nitrogen respectively), or as fine powders such as TiO_2 to provide a metal source.

The plasma is contained in a quartz tube which is fed by three coaxial inlet flows. The outermost flow is the sheath gas. It surrounds the plasma with cool gas to protect the walls of the containment tube and it has a tangential swirl component to help stabilize plasma oscillations. The middle flow is used to introduce the reactant plasma gases. The solid particles are introduced in the third, central flow. The solid reactants are typically 50 to 100 μm particles that are suspended in a carrier gas. The carrier gas is usually a mixture of inert gas and a reactive gas.

Once the plasma has been initiated, energy is supplied to the system through Ohmic heating. Electron motion is induced in the fluctuating field in the RF coil and energy is redistributed throughout the system via electron-molecule collisions. At the temperatures and pressures in this system, electron temperatures and ion and neutral temperatures are equal and the system is in local thermodynamic equilibrium. Peak temperatures in the system are typically off center because of the shielding effect of the ionized gases.

The plasma is characterized by high temperature and velocity gradients as well as large variations in properties concomitant with the large temperature variations. Temperatures vary from room temperature to approximately 10,000 K. Velocity gradients are caused by the large change in density associated with heating the gas. While velocity gradients are large due to the property variations, typical velocities are only on the order of several meters per second and Reynolds numbers based on the containment tube diameter range between approximately 300 and 700. The Reynolds numbers remain relatively low throughout the whole torch because of the increase in viscosity and decrease in density with increasing temperature, (see Figure 2).

Residence times in the plasma are on the order of 10 ms. Because of these short residence times and the large temperature and velocity gradients, incomplete vaporization of solid reactants is one of the limiting factors in plasma processing. If the solid particles do not pass through the hottest part of the plasma, then the material may not be fully vaporized and the product quality will be low. Because of the swirling of the sheath gas, the three coaxial flows and the large density gradients, plasma flows are often characterized by recirculation and very sharp changes in direction of the gas streamlines. The streamline paths are not obvious and particles may slip in the flow where there are sharp directional changes. Because of this, it is difficult to know where to inject the particles to get them to pass through the hotter parts of the plasma to ensure good vaporization.

It is difficult to make measurements in plasmas during operation. Normal diagnostic techniques such as laser velocimetry are hard to apply because of the intense heat and

Table I. Base case operating conditions

Q_1 =	3.6	l/min	frequency =	13.5	MHz
Q_2 =	1.15	l/min	coil	4	turns
Q_3 =	17.9	l/min	I	100	Amps
Total	22.65	l/min	Power	3.0	kW

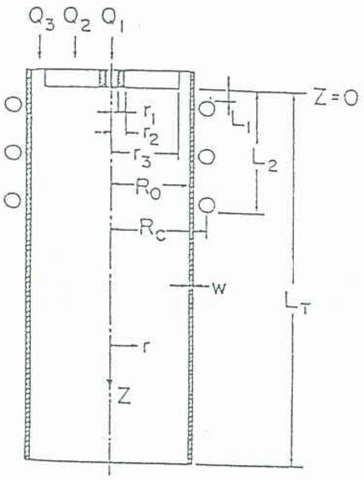


Figure 1. Dimensions of the RF plasma torch

r_1 =	1.0	mm	L_1 =	0.0	mm
r_2 =	5.0	mm	L_2 =	42.0	mm
r_3 =	12.25	mm	L_T =	138.0	mm
R_o =	21.0	mm	w =	2.0	mm
R_c =	27.7	mm			

the luminosity of the plasma. Variations in reactants and system parameters also mean that results from one system are not necessary applicable to another plasma system. Because of these difficulties, numerical modeling is becoming a powerful tool to help in the design of plasma systems.

A number of groups have modeled plasma torches in recent years. The most recent of these efforts have looked at modeling of the flow and temperature fields for two-dimensional flows with two dimensional electromagnetic fields (Mostaghimi et al., 1984; Mostaghimi et al., 1985; Mostaghimi and Boulos, 1989; Chen and Pfender, 1991). The model in this work extends the geometry to a quasi-three dimensional case to include the effect of swirl on the system. The large degree of swirl induced in the sheath gas to stabilize the plasma is shown to have an important influence on the system.

NUMERICAL MODEL

Because of the complexity of the system a number of simplifying assumptions were made in the model. The electromagnetic field equations were reduced to one dimension. This assumption is possible when the length to diameter ratio of the coil is greater than one and end effects are of second order, (Mostaghimi and Boulos, 1989). The wavelength of the RF field is much larger than the length of the torch so the displacement current in Maxwell's equations could also be neglected compared to the conductive current. The torch operates at one atmosphere pressure. With the given RF frequency, the system may be assumed to be in local thermodynamic equilibrium so that there is one characteristic temperature for ions, electrons and neutrals. The plasma was considered to be optically thin, i.e., none of the radiation emitted was re-absorbed by the gas in the system. The plasma gas is assumed to be argon. (In actual practice the gas flow through the system is typically only 5 to 10 percent reactant gas and the rest is argon.)

The assumptions can be listed as:

a. Axisymmetric, 2-D temperature field.
b. Axisymmetric, steady state, laminar, quasi-3-D flow field.
c. Axisymmetric 1-D electromagnetic fields.
d. Local thermodynamic equilibrium.
e. Optically thin plasma
f. Negligible displacement currents.

The descriptive equations can be written in the following forms;

Continuity

(1)
$$\frac{1}{r}\frac{\delta}{\delta r}(\rho r v_r)+\frac{\delta}{\delta z}(\rho v_z)=0$$

Momentum

(2)
$$\rho\left(v_r\frac{\delta v_z}{\delta r}+v_z\frac{\delta v_z}{\delta z}\right)=$$
$$-\frac{\delta p}{\delta z}+2\frac{\delta}{\delta z}\left(\mu\frac{\delta v_z}{\delta z}\right)+\frac{1}{r}\frac{\delta}{\delta r}\left[\mu r\left(\frac{\delta v_z}{\delta r}+\frac{\delta v_r}{\delta z}\right)\right]$$

(3)
$$\rho\left(v_r\frac{\delta v_r}{\delta r}-\frac{v_\theta^2}{r}+v_z\frac{\delta v_r}{\delta z}\right)=-\frac{\delta p}{\delta r}$$
$$+\frac{2}{r}\frac{\delta}{\delta r}\left(\mu r\frac{\delta v_r}{\delta r}\right)+\frac{\delta}{\delta z}\left[\mu\left(\frac{\delta v_r}{\delta z}+\frac{\delta v_z}{\delta r}\right)\right]-\frac{2\mu v_r}{r^2}+F_r$$

(4)
$$\rho\left(v_r\frac{\delta v_\theta}{\delta r}+\frac{v_r v_\theta}{r}+v_z\frac{\delta v_\theta}{\delta z}\right)=$$
$$\frac{1}{r^2}\frac{\delta}{\delta r}\left[r^2\mu\left(\frac{\delta v_\theta}{\delta r}-\frac{v_\theta}{r}\right)\right]+\frac{\delta}{\delta z}\left(\mu\frac{\delta v_\theta}{\delta z}\right)$$

Energy

(5)
$$\rho\left(v_r\frac{\delta h}{\delta r}+v_z\frac{\delta h}{\delta z}\right)=\frac{1}{r}\frac{\delta}{\delta r}\left(r\frac{k}{C_p}\frac{\delta h}{\delta r}\right)+\frac{\delta}{\delta z}\left(\frac{k}{C_p}\frac{\delta h}{\delta z}\right)+P-Q_r$$

Magnetic Field Equations

(6) $\frac{1}{r}\frac{d}{dr}(rE_\theta)=-\xi\omega\sin\chi$ (7) $\frac{dH_z}{dr}=-\sigma E_\theta\cos\chi$

(8)
$$\frac{d\chi}{dr}=\frac{\sigma E_\theta}{H_z}\sin\chi-\frac{\xi\omega H_z}{E_\theta}\cos\chi$$

The volumetric rate of heat generation in the plasma due to Ohmic heating is;

(9)
$$P=\sigma E_\theta^2$$

The electromagnetic heat source term varies as a function of radius because the electrical conductivity of the ionized gas tends to shield the gas near the center of the torch. This also tends to give an off center temperature peak in the system.

The electromagnetic body force acting on the gas in the discharge region is given by;

(10)
$$F_r=-\xi\sigma E_\theta H_z\cos\chi$$

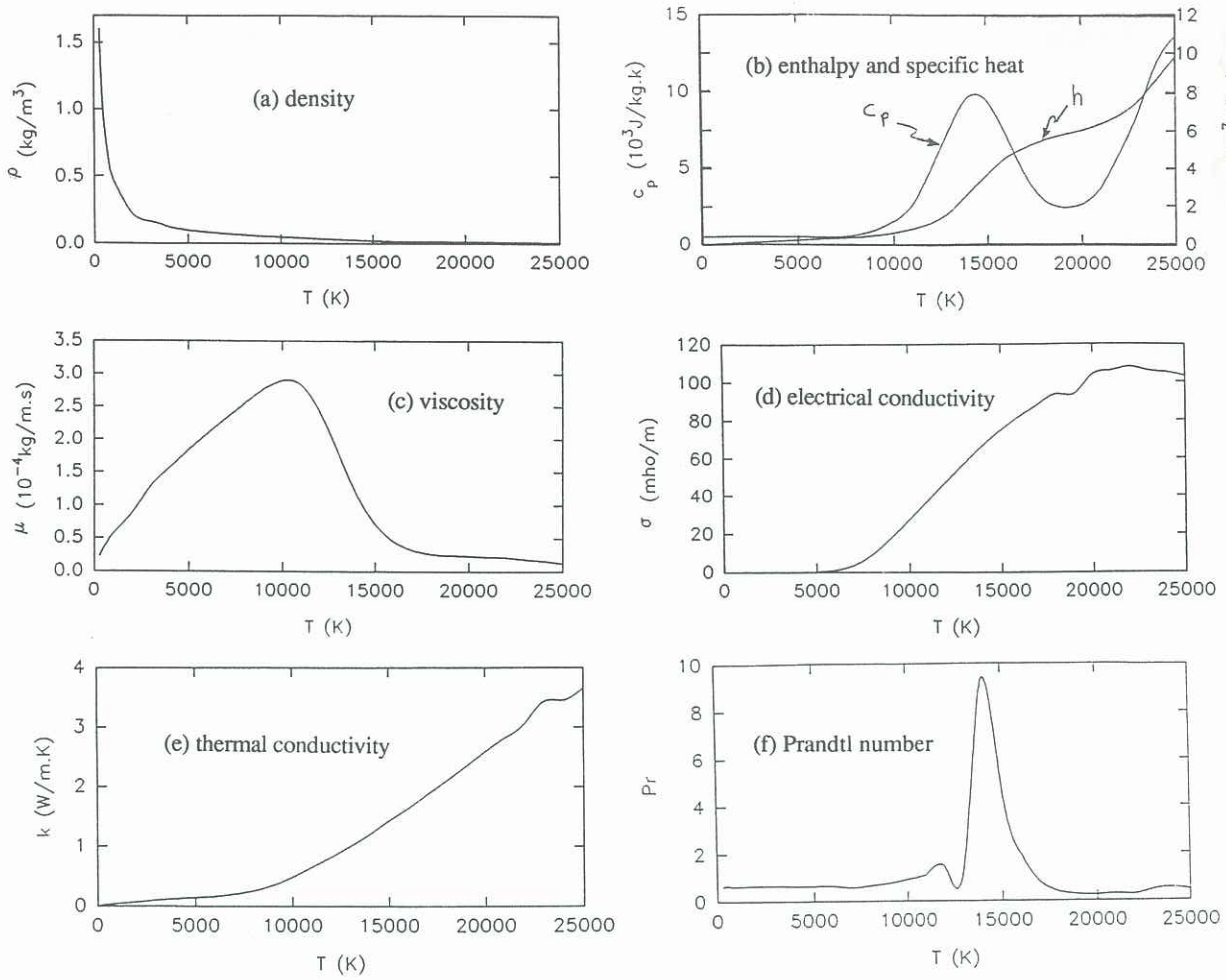


Figure 2. Properties of Argon versus temperature. (a) density, (b) enthalpy and specific heat, (c) viscosity, (d) electrical conductivity, (e) thermal conductivity, (f) Prandtl number.

The energy equation has been written in terms of the specific enthalpy and the temperature at any point may be recovered from the relation;

(11)
$$T = -288.24 + 2.6775 * 10^{-3} h - 1.1635 * 10^{-10} h^2$$

The inclusion of the swirl component, V_θ, is a departure from the standard treatment of plasma torch modeling. While there are some full three dimensional effects due to the fact that the gas is introduced through a series of individual holes arrayed in concentric circles, the standard approach is to assume that the gas enters through a ring with a cross sectional area equal to the combined area of the injection holes, (Chen and Pfender, 1991).

The model with swirl is considered to be as complete as possible without moving to a full 3-D analysis.

Boundary conditions

Inlet (z = 0)

(12)
$$v_r = 0$$
$$v_z = \frac{Q_i}{\pi\left(r_{i-out}^2 - r_{i-in}^2\right)} \quad \text{where there is flowing gas}$$
$$v_z = 0 \quad \text{otherwise}$$
$$v_\theta = v_{inlet}\sin(\text{injection angle})$$

Centerline (r = 0)

(13)
$$v_r = 0 \qquad \frac{\delta v_z}{\delta r} = 0 \qquad v_\theta = 0$$

Wall (r = R₀)

(14)
$$v_r = v_z = v_\theta = 0 \qquad \frac{k}{C_p}\frac{\delta h}{\delta r} = \frac{k_c}{w}\left(T - T_{wo}\right)$$

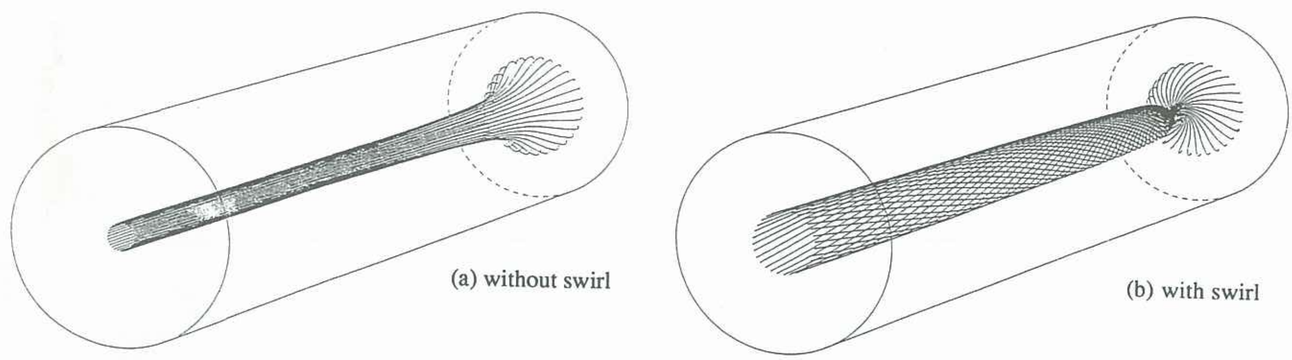
Exit (z = L_T) It is assumed that flow is fully developed at the exit and that gradients of velocity, mass flow and enthalpy in the axial direction are relatively small and can be taken as zero. In order to make this assumption, calculations are carried out for several diameters past the plasma to remove the effect of exit conditions from the behavior of the plasma in the region of interest.

(15)
$$\frac{\delta v_r}{\delta z} = 0 \qquad \frac{\delta(\rho v_z)}{\delta z} = 0 \qquad \frac{\delta h}{\delta z} = 0 \qquad \frac{\delta v_\theta}{\delta z} = 0$$

The electromagnetic field boundary conditions for the magnetic equations at r = 0 and $L_1 < z < L_2$ are;

(16)
$$E = 0 \qquad \chi = \pi/2$$

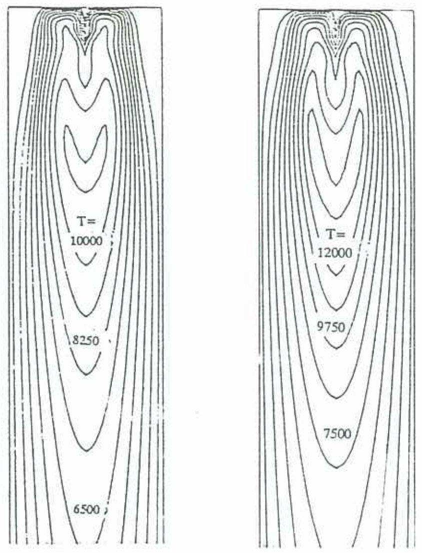
$$H_z = \frac{NI}{(L_2 - L_1)}\left\{\frac{L_2 - z}{\left[R_c^2 + (L_2 - z)^2\right]^{1/2}} - \frac{L_1 - z}{\left[R_c^2 + (L_1 - z)^2\right]^{1/2}}\right\}$$



(a) without swirl

(b) with swirl

Figure 3. Streamlines for the base case plasma torch. (Streamlines start at $r = 0.5\ R_o$)



(a) without swirl

(b) with swirl

Figure 4. Isotherms for the base case plasma torch conditions

The fluid mechanic continuum equations, (1 to 5), were solved numerically using a finite volume method on an r,z mesh. The mesh had non-uniform spacing in the z direction to capture the details of the flow in the inlet region. The electromagnetic field was solved by Runge-Kutta integration of equations, (6 to 8). The electromagnetic equations were coupled to the continuum equations via the energy dissipation term, equation (9), and the body force term, equation (10). The Runge-Kutta integration was imbedded into the fluid dynamics solver. The PHOENICS package provided the framework for solving the continuum equations with the Runge-Kutta code being incorporated in a purpose built PHOENICS "ground" subroutine.

In modeling plasma systems, one of the difficulties that must be handled is the extreme variations in fluid properties. Data for the thermodynamic and transport properties were calculated by Dr. Tony Murphy of CSIRO, Lindfield, Australia. The properties are shown as function of temperature in Figures 2(a) to 2(f). The most notable features are the effect of ionization on the enthalpy and specific heat of the gas (Figure 2(b)), and the sudden increase in conductivity with the beginning of ionization around 7500 K and its effect on the thermal and electrical conductivities of the gas (Figures 2(d) and 2(e)). The sharp peak in the Prandtl number (Figure 2(f)) is due to the large energy associated with the essentially complete first ionization of argon.

RESULTS AND DISCUSSION

A base case for the torch operating at the University of Auckland was run with a number of different combinations of variable density, Prandtl number (thermal conductivity, specific heat and viscosity) and electrical conductivity to determine the sensitivity of the system to the variables. The results showed that the electromagnetic body force tends to increase recirculation and steepen the temperature gradients. The variation in density causes the flow to travel farther before it becomes fully developed and the temperature gradients become sharper. Allowing variation in Prandtl number results in higher peak temperatures. Overall, the strongest effect was the variation in density. At higher temperatures, density variation includes contributions due to the increase in mole number due to ionization.

The effect of swirl on the system is shown in Figures 3 and 4. Figure 3 shows the isotherms for the cases with and without swirl; there is little difference in the temperature profiles between the two. However, Figure 4 shows streamlines for the two cases, where there is clearly a marked difference as far as recirculation and particle trajectories through the flow are concerned. Swirl must be included to accurately model particle trajectories through the plasma torch system.

The ability to track streamlines is important because it can be used to understand the nature of the flow and how to best inject particles for vaporization. Qualitatively, the numerical model results compare well with observed behavior of the torch the program was meant to model. If particle streamlines can be followed through the various temperature and flow fields, then a temperature time history for the particle can be extracted from the data and analytical techniques used to estimate percentage of vaporization or alternatively maximum particle sizes for vaporization. This capability is currently being developed. The handling and feeding of micron size powders is difficult. The ability to use larger particles in the system would reduce the materials handling requirements. This work is of general interest because many plasma processes rely on the vaporization of solid particles to introduce some of the reactants into the system.

Future work will include extending the flow field calculations to a full 3-D representation in order to more accurately model the effects of inlet nozzle sizes and distributions, and the electromagnetic fields will be extended to the 2-D case for a more accurate representation of the end effects in the RF coil.

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