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Effect of Shroud gas Injection on Thermal and Fluid Behavior of RF Plasma Reactor used for Nanosynthesis of Alumina

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Abstract: **A 2D model for the simulation of inductively coupled RF plasma torches (ICPTs) working at atmospheric pressure used for Nanosynthesis of Alumina (Al_2O_3) is presented, using a customized version of the computational fluid dynamics (CFD) commercial code FLUENT®. Steady state, continuity, momentum and energy equations are solved for optically thin argon plasmas under the assumptions of local thermodynamic equilibrium (LTE) and laminar flow. The electromagnetic field equations are solved on an extended grid in the vector potential form outside the torch. In order to evaluate the importance of various 2D effects on calculated plasma temperature and velocity fields. The effect of changing positions of sheath gas inlet and central gas inlet on the temperature and velocity flow pattern are discussed.**

Keywords: **plasma torches; CFD, Nanosynthesis, plasma simulation; high-frequency; rf discharges.**

1. INTRODUCTION

Thermal plasma synthesis of nanopowders through Evaporation, quenching, and nucleation using radio Frequency (RF) or arc plasma sources is a well-establishedtechnique for mass production of novel nanomaterials[1]–[6]. While inductively coupled plasma (ICP) reactors areroutinely used in semiconductor industries for low-pressureplasma processing, atmospheric pressure RF thermal plasmasources are gaining increasing importance in production ofhigh purity novel nanomaterials in different high-end technologicalapplications.

Synthesis of nanoparticles through thermal evaporation andcondensation is of interest to the researchers for a longtime. Kimoto *et al*. [7] synthesized aluminum nanoparticlesthrough evaporation in argon at low pressures in the early1970s. Study of plasma particle interaction ininduction plasma became important as it was observed that inmany cases, the powder particles injected from the top of theplasma torch bounce off the induction plasma ball and do notenter the higher temperature zones inside [8]Mathematical modelling is a powerful tool to deeply investigatePhysical and chemical phenomena occurring withininductively coupled plasma torches (ICPTs). Various numericalmodels of increasing complexity have been proposedover the years with the aim of obtaining a more andmore realistic prediction of plasma behavior and chemicalprocesses inside the torch. Current state of the art inthis research field includes the fully 3-D description of thesystem, as recently performed by the authors by meansof either complete [9] or simplified [10] approaches for thetreatment of the electromagnetic field.

Nevertheless, two-dimensional axisymmetric modelsare still widely used for calculating the plasma temperature, flow and concentration fields in ICPTs. In this regard, many efforts have been devoted in the last yearsto continuously improve 2-D models, *e.g.* by taking intoaccount also turbulence phenomena [11] or including someimportant 3-D effects due to the non-axisymmetric shapeof the induction coil [12].

In addition to the improvement of 2-D models, muchwork has been done to suitably customize the CFD Commercial code FLUENTfor simulating RF thermalplasma sources. FLUENToffers important advantagesin modelling, such as the possibility of studying complicatedgeometries, using different physical and numericalmodels and easily generating both structured and unstructuredmeshes. The need for customizing the basic code liesin the fact that, by default, the FLUENT c_ built-in solvercan only treat mass, momentum and energy conservationequations, but it does not include any computational modulefor solving the electromagnetic field equations involvedin the modelling of induction plasmas.To overcome this difficulty, Bouloset al. [12, 13] exploitthe

FLUENT feature which allows one to add new userdefinedscalars (UDS) to the variables basically employedby the built-in solver. In particular, they define two UDSfor the real and imaginary parts of the complex vectorpotential and then let the FLUENTroutines solve thecorresponding governing equations. This approach is quitesimple to implement but has some numerical drawbacksdue to the intrinsic customization limits of the software.In fact, FLUENT requires all the equations of the modelto be solved on the same domain, which implies that eventhe computation of the fluid dynamic variables must beextended outside the torch region when a far field approachis used for the treatment of the electromagneticsof the system. This might result in numerical unstabilitiesand/or slow convergence of the solution process. To overcome this difficulty D. Bernardi exploit the FLUENTfeature which allows one to add new user defined function (udf) (14).

2. EXPERIMENTAL SYSTEM

A schematic of the Nanosynthesis system used in this paperis shown in Fig. 1. It consists of a gas supply system, highvoltagedc power supply unit feeding an oscillator circuit, powder feeder unit, RF plasma torch, primary depositionchamber, gas cooling chamber, cooling coils, cyclone separator, filter cartridge assembly, and a vacuum pump unit. TheRF generation unit consists of a high-voltage power supply (12 kV–10 A) unit.

The reaction chamber consists of an RF plasma tube on the top of a cylindrical SS chamber. The SS chamber is connected to a horizontal extension chamber fitted with water cooled coils for further cooling of the flowing gas and deposition of particles. After this chamber the relatively cooler gas passes through a cyclone separator for settling down the remaining particles and finally goes out into the atmosphere after passing through an assembly of metallic filter. A pneumatically controlled root pump connected with the system can reduce the pressure of the reaction chamber up to 50 mbar and set the chamber pressure at any desired value between 50 mbar and 1 bar. A chilled water supply system fitted with a heat exchanger unit appropriately cools the system. The RF plasma tube is a double walled glass cylinder with an inner bore of 60 mm and length 465 mm.

Cooling water runs from bottom to the top of the torch through the space between the inner and the outer wall and removes the heat deposited on the glass wall by plasma during operation. While the particle carrier gas is injected exactly along the axis of the torch through a relatively long tube, there is an aerodynamically designed multiport gas distribution system for plasma gas, sheath gas on the top of the plasma tube. The carrier gas is fed exactly at the center of the tube, the plasma gas is fed little off center and the sheath gas is fed near the inner edge of the plasma tube with a swirl. While the plasma gas forms the plasma, the sheath gas confines the produced plasma in the middle of the plasma tube and thereby avoids direct contact of the plasma with the glass wall. A powder feeder unit, similar to those used in typical plasma spray setup, is connected to the carrier gas port of the plasma tube. The feeder unit has a rotor disk whose rotation speed can be set to a predecided value. Feed rate of the powder into the plasma depends on rotation speed of the rotor disk. Thefluidized powder enters exactly into the middle of the plasma column through a long metallic tube and gets instantaneously evaporated to form plasma in the prevailing strong thermal field. Typical operating parameters during operation of the plasma are shown in Table I.

To ignite the system, initially the root pump is switched on, all gas inlets are closed and the base pressure is brought down to 50 mbar. Plasma gas is set to 5 slm (this shifts base pressure to 63 mbar), grid voltage, and filament current are set as in Table I. As RF voltage and current are increased

TABLE I

OPERATING PARAMETERS FOR THE SYNTHESIS OF NANOPHASE α-ALUMINA

Item	Description	Item	Description
1. Plasma Gas	Argon	7. Coil current	4.5 A
2. RF Frequency	3 MHz	8. Filament current	165 A
3. RF Voltage	4 KV	9. Grid Voltage	11 V
4. Rotor Speed	6.57 rpm	10. Sheath Gas Flow	10 slm
5. Plasma Gas Flow	15 slm	11. Carrier Gas Flow	15 slm
6. Powder feed rate	400gm/hr		

in unison, a plasma glow starts which finally settles into an extremely luminous plasma column as voltage and current are set as in the above table. Sheath gas is put on and plasma gas is increased to the set value. Gas pressure is gradually increased to atmospheric pressure and vacuum pump is turned off. The plasma luminosity increases many fold. Now the carrier gas is set and powder feed starts as in Table I. Copious nanoparticles starts forming and get deposited on the plasma tube wall and everywhere inside the bottom chamber as well assubsequent cooling sections [Fig. 1]. Finer powdersare carried forward into the cooling chamber and get deposited over the cooling coils and side walls. Furthermore, finer powders moves forward and get deposited at the bottom of the cyclone chamber. The gas then passes through a multilayered metallic filter before finally getting discharged into the atmosphere. RF plasma tube with nanoparticles deposited over the inner wall, inside view of the plasma tube with thick layer of deposited particles, dome of nanoparticles created at the bottom of the reaction chamber. Once a run is over, the deposited particles are collected, labeled, and stored.

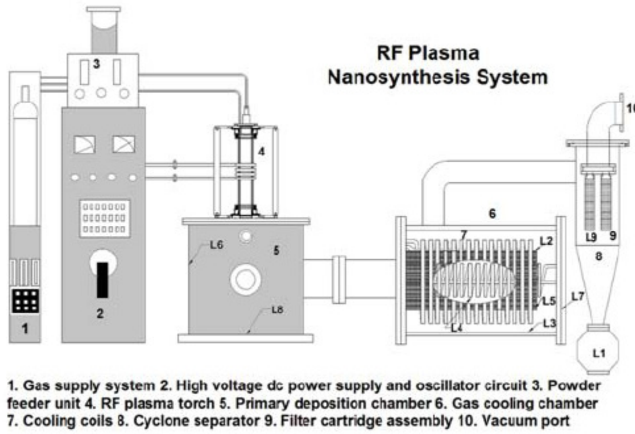


Fig 1. Experiment set up

3. MODELLING APPROACH AND CFD EQUATIONS

The following basic assumptions have been adopted throughout this work:

1. The torch is represented by a fully axisymmetric configuration;

2. The plasma is assumed to be optically thin and in local thermodynamic equilibrium (LTE) under atmospheric pressure conditions;

3. The flow is laminar and the tangential component of plasma velocity is not taken into account;

4. Viscous dissipation and pressure work in the energy equation are neglected;

5. Displacement current associated with the oscillatory magnetic field is assumed to be negligible.

Because the FLUENT software was used to implement the present model, the Navier-Stokes equations do not require any special consideration since they are integrated in the solver. The default energy equation (expressed in terms of temperature within FLUENT) was deactivated and replaced by a scalar for enthalpy h. This change was performed in order to overcome the limited formula available within FLUENT for the specific heat, that must be integrated in the case of a temperature formulation.

In the case of a two-dimensional axisymmetric coordinate system (x, r, h), the conservation equations may be written as:

Continuity

$$\frac{\partial(\rho u)}{\partial x}+\frac{1}{r}\frac{\partial(r\rho v)}{\partial r}=0 \qquad (1)$$

Axial momentum

$$\rho\left[\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial r}\right]=-\frac{\partial P}{\partial x}+2\frac{\partial}{\partial x}\left[\mu\frac{\partial u}{\partial x}\right]+\frac{1}{r}\frac{\partial}{\partial r}\left[r\mu\left(\frac{\partial u}{\partial r}+\frac{\partial v}{\partial x}\right)\right]+\rho g+F_{\mathrm{LX}} \qquad (2)$$

Radial momentum

$$\boldsymbol{\rho\left[\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial r}\right]=\frac{\partial P}{\partial x}+\frac{\partial}{\partial x}\left[\mu\left(\frac{\partial v}{\partial x}+\frac{\partial u}{\partial r}\right)\right]+\frac{2}{r}\frac{\partial}{\partial r}\left[r\mu\frac{\partial v}{\partial r}\right]-\frac{2\mu v}{r2}+\rho\frac{w2}{r}+F_{Lr}} \qquad (3)$$

Swirl momentum

$$\rho\left[u\frac{\partial(rw)}{\partial x}+v\frac{\partial(rw)}{\partial r}\right]=\frac{\partial}{\partial x}\left[\mu\left(\frac{\partial(rw)}{\partial x}\right)\right]+\frac{1}{r}\frac{\partial}{\partial r}\left[r\mu\frac{\partial(rw)}{\partial r}\right]-\frac{2}{r}\frac{\partial}{\partial r}(\mu rw) \qquad (4)$$

Enthalpy:

$$\rho\left[u\frac{\partial h}{\partial x}+v\frac{\partial h}{\partial r}\right]=\frac{\partial}{\partial x}\left[\frac{k}{cp}\frac{\partial h}{\partial x}\right]+\frac{1}{r}\frac{\partial}{\partial r}\left[r\frac{k}{cp}\frac{\partial h}{\partial r}\right]+qJ-qr \qquad (5)$$

Boundary conditions for Eqs. (1)–(5) are as follows:

(I) $x=0$ (at the torch inlet):

$$v=0,\qquad h=h_0 \text{ (corresponding to 350 K)}$$

$$\begin{cases} u=\dfrac{Q_1}{(\pi r_1^2)}, & rw=0, \quad \text{for } r\le r_1 \\ u=0, & rw=0, \quad \text{for } r_1\le r\le r_2 \\ u=\dfrac{Q_2}{\pi(r_3^2-r_2^2)}, & rw=ru, \quad \text{for } r_2\le r\le r_3 \\ u=0, & rw=0, \quad \text{for } r_3\le r\le R_0 \end{cases} \qquad (6)$$

(II) $x=L_T$ (at torch exit); one-way boundary conditions will be used:

$$\frac{\partial u}{\partial x}=v=\frac{\partial(rw)}{\partial x}=\frac{\partial h}{\partial x}=0 \qquad (7)$$

(III) $r=0$ and $x>L_{\mathrm{tube}}$:

$$\frac{\partial u}{\partial r}=v=rw=\frac{\partial h}{\partial r}=0 \qquad (8a)$$

$r=r_{\mathrm{tube}}$ and $x\le L_{\mathrm{tube}}$:

$$u=v=rw=0,\qquad h=h_{\mathrm{tube}} \text{ (corresponding to 500 K)} \qquad (8b)$$

(IV) $r=R_0$ (torch wall):

$$u=v=rw=0 \qquad -\left[\frac{k}{C_p}\frac{\partial h}{\partial r}\right]_w=\frac{\kappa}{\delta}(T_{wi}-T_{wo}) \qquad (9)$$

in which q, l, j, and Cp stand for density, dynamic viscosity, thermal conductivity, and specific heat, respectivelyand u, v, and x are the axial, radial, and swirl velocitycomponents, respectively.

The corresponding one dimensional electromagnetic field equations are

$$\frac{1}{r}\frac{d}{dr}(rE\theta)=-\int\omega Hzsin$$

$$\frac{dHz}{dr} = -\sigma E\theta cosx$$

$$\frac{dX}{dr} = \frac{\sigma E\theta}{Hz} sinX - \frac{\int\omega Hz}{E\theta} cosX$$

Where Fr=$-\int\omega Hz$cosX is radial body force acting on plasma gas in discharge region and the boundary conditions are same as above.

4. RESULTS AND DISCUSSION

In spite of many advantages offered by the FLUENT code for studying complex fluid dynamic phenomenaits use in the modelling of inductive plasmas is notstraightforward. This is due to the fact that, at present, FLUENTsolves, by default, only mass, momentum and

Energy conservation equations but does not provide anybuilt-in module for EMfield calculations. To overcome thisdifficulty the UDF is generated.

For the simulation geometry is as follows

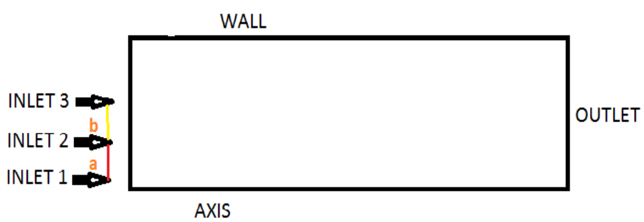


Fig. 2. Geometry

For simulation there are six cases which are follow

Case l: a=b=5mm

Case ll : a=b=5mm, inlet 2&3 with swirl 30 degree

Case lll : a=b=5mm, inlet 2&3 with swirl 45 degree

Case lV: a=b=10mm

Case V: a=b=10mm, inlet 2&3 with swirl 30 degree

Case VI: a=b=10mm, inlet 2&3 with swirl 45 degree

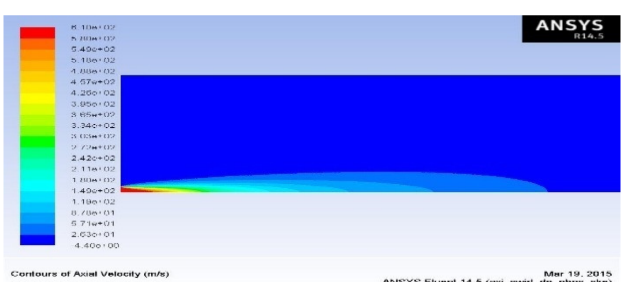


Fig 3. Temperature profile

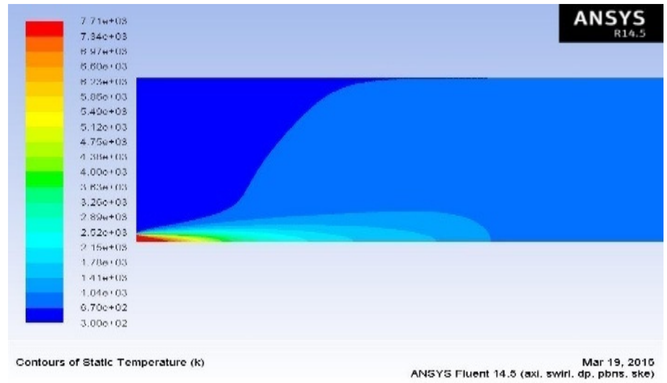
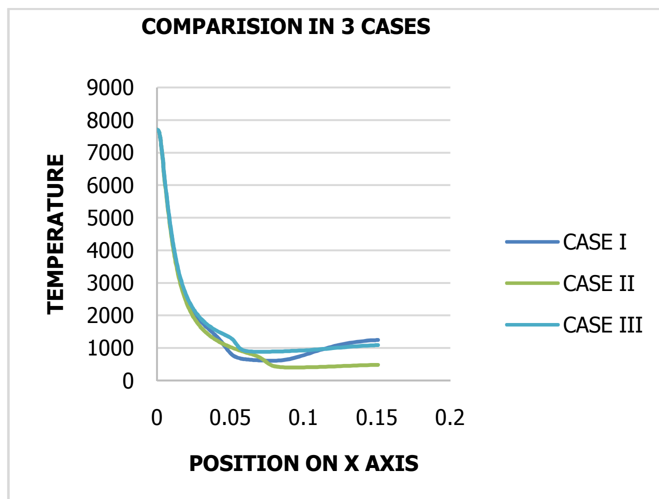
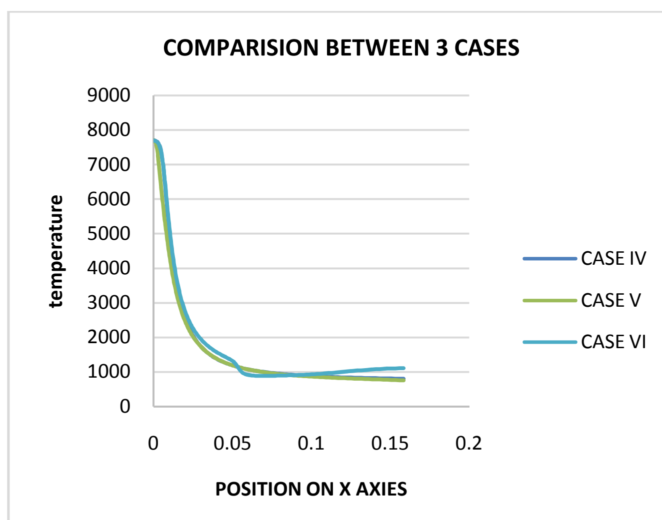
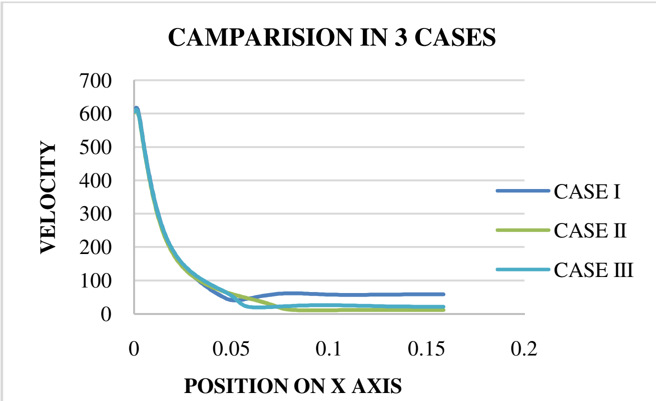


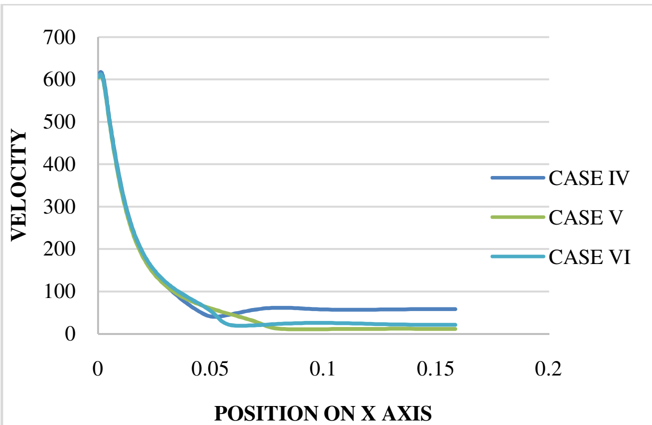
Fig. 4. Velocity profile

The temperature profile and velocity profile for all cases are same but there is difference in high temperature and high velocity zone. This is seen in graphs.









The highest temperature exhibited by the zoneis sufficient for instantaneous evaporation of the micrometersized particles. The steep gradient in the downstream zoneimmediately after it leads to rapid quenching and formationof nanometer-sized particles. Considering large volume of theRF plasma, obtained distribution of axial temperature mayinclude some errors depending on validity of the opticallythin assumption. It should be pointed out that the temperatureprofile so measured without powder injection may be modified

to some extent depending on feed rate. However, as far aspossible gradient in temperature is concerned, even the measurementwith pure argon plasma can offer a good trend. Thisis because the ultimate temperature gradient is primarily set bythe facilitated external channels for heat removal, which do notget drastically modified for the powder feed rates considered.

5. CONCLUSION

A CFD model of a high-frequency ICP was developedin order to obtain a better knowledge and understanding

of the nanoparticle synthesis process. This model considers the couplingbetween electromagnetic and Navier-Stokes equationsand was implemented in the FLUENT software by usingUser Defined Functions (UDFs) written in C language.The contribution of the magnetic part was formulated interms of vector potential on the basis of a one-dimensionalaxisymmetric assumption and an extended field of calculationwas considered. The model permits to quantify theinfluence of the more relevant parameters such as the gasflow rates, the current frequency, the working pressure, the power input, etc. on the plasma flow and on the maincharacteristic fields such as velocity and temperature.The peak velocity and temperature of geometry having swirl to inlets is greater than other geometries.

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