Numerical simulation of the argon-hydrogen plasma flow in the channel of RF inductively coupled plasma torch

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Abstract. The results of numerical simulation of plasma flow in the channel of technological radio frequency (RF) plasma torch with three coils and frequency at 3 MHz are presented. The mixture of argon with hydrogen is considered as the working gas at a variation of hydrogen volume fraction $\alpha$ from 0 to 10%. The distributions of electromagnetic fields and gas-dynamic parameters of the plasma flow are calculated. It is shown that when the amplitude of discharge current exceeds the critical value $J_{cr}$ (depends on $\alpha$), the regime of plasma flow transforms from the potential to vortical regime, in which a toroidal vortex is formed before or in the inductor zone. The dependence of the values of the critical current $J_{cr}$ on the volume concentration of hydrogen $\alpha$ is established. The influences of volume fraction $\alpha$ and discharge current $J_{coil}$ on the intensities and the position of the vortex center are determined.

1. Introduction
At present in connection with the development of new technologies for the production of ultrapure substances [1-8], nanopowders [9, 10], the interests in the inductively coupled plasma (ICP) torch are steadily increasing [11-13]. The basic gas–dynamic parameters (velocity and temperature) are determined by the flow regimes in the inductor zone (exothermic zone). Results [12-17] indicate that there is a specific vortical flow regime in this zone under high discharge current. This leads to the change of gas flow pattern and has a negative impact on plasma processing of solid particles, because it prevents the injected solid particles from penetrating deeply into the high temperature plasma region.

The implementation of plasma technologies requires various different kinds of working gases, among which the mixture argon with different hydrogen volume fractions is considered in our studies. The purpose of this work is to investigate the plasma flow regimes in the ICP plasma torch, find the conditions of forming vortex and determine the parameters of the vortex flow under different hydrogen volume fractions.

2. Physical and mathematical model.
The numerical simulations of an RF ICP plasma torch with axial gases supplies (Fig. 1) and three inductor coils are studied. The copper coils with a wire diameter $d_{coil}=6$ mm and winding radius $R_{coi}=33$ mm is evenly distributed. The first coil is located at $Z_{coi}=63$ mm. The distance between the first and the last coil is set at $l_{in}=l_{out}=60$ mm. The amplitude of discharge current $J_{coil}$, varying sinusoidally with frequency $\omega = 3$ MHz, is chosen in the range of 80-300 A.
The mass flow rates of transporting, central and sheath gases are correspondingly set at \( G_1 = 0.87 \times 10^{-6} \) kg/s, \( G_2 = 1.02 \times 10^{-8} \) kg/s and \( G_3 = 1.41 \times 10^{-7} \) kg/s. The central transporting probe with an internal radius \( R_1 = 1.7 \) mm and wall thickness \( \delta_1 = 2 \) mm is fixed at \( Z_1 = 50 \) mm.

Figure 1. Scheme and geometric parameters of the ICP plasma torch: 1 – injection probe of transporting gas and quartz particles, 2 – channel of central gas, 3 – channel of sheath gas.

The length of external quartz channel is \( Z_4 = 400 \) mm with an internal radius \( R_3 = 25 \) mm and wall thickness \( \delta_3 = 3.5 \) mm. The peripheral slit channel is also located at \( Z_2 = 50 \) mm with a width \( R_3 - R_2 = 2.2 \) mm.

In the present calculations the spiral inductor is assumed as three cylindrically symmetric parallel coils. The flows of transporting, central and sheath gases at the inlets are azimuthally symmetrical and stationary. Under the fulfillments of these assumptions the electromagnetic and gas dynamic equations can be written under 2D – model in the cylindrical coordinate \((r, z)\) system. It is calculated that plasma flow in the ICP channels is laminar and subsonic with average \( Re \) number \( Re < 1000 \).

The gas dynamic parameters of the plasma flow are calculated on the basis of plasma dynamic system equations, including Maxwell equations (without displacement current) and gas dynamic equations. The effect of electromagnetic forces and Joule heating in the plasma dynamics equations have been taken into accounted.

The Maxwell equations (1) (displacement current is neglected) are written via the magnetic vector potential [15]:

\[
v^2 \vec{A} = -\mu_0 (j_{col} + j_{ind}), \tag{1}
\]

where \( j_{col} \) is the vector of discharge current density in the coils from the RF power supply, \( j_{ind} \) is the vector of induced current density in the plasma region and in the coils [11, 16]. Note that under the assumptions of cylindrical symmetry the vector potential \( \vec{A} \) and \( j_{col} \) have only a \( \theta \) –tion component (varying sinusoidally with frequency \( \omega = 3 \) MHz). The electric, magnetic field and the induced current are calculated by formula (2):

\[
\begin{align*}
B_r &= -\frac{\partial A_\theta}{\partial z}, \\
B_z &= -\frac{\partial}{\partial r} (r A_\theta), \\
E_\theta &= -i \omega A_\theta, \\
J_\theta &= \sigma E_\theta = -i \sigma \omega A_\theta, \tag{2}
\end{align*}
\]

where \( \sigma(T) \) is the electrical conductivity of argon–hydrogen plasma.

The system of plasma dynamic equations [16] is written in formula (3–5), taking into account of the electromagnetic forces and Joule heating (the radiation loss energy is negligible).

\[
\begin{align*}
\nabla \cdot (\rho \vec{U}) &= 0, \tag{3} \\
\nabla \cdot (\rho \vec{U} \times \vec{B}) &= -\nabla P + j_{EM} + \nabla \cdot (\lambda \nabla T) + q_v, \tag{4} \\
\n\nabla \cdot (\rho \vec{U}) &= \nabla \cdot (\lambda \nabla T) + q_v, \tag{5}
\end{align*}
\]

where \( \mu, \lambda \) are the dynamic viscosity and thermal conductivity of plasma gas; \( j_{EM}, q_v \) are the volumetric sources of electromagnetic force and joule heating, which are calculated by formula (6):

\[
\begin{align*}
\nabla \cdot (\rho \vec{U}) &= \sigma \Re (E_\theta B_z^* + \Re (E \vec{E}^*)) \tag{6},
\end{align*}
\]

where \( E^* \) and \( B^* \) are the complex conjugate of \( E \) and \( B \).

The boundary conditions for (1–3) equations are given as that: the velocities of gases at the walls are zero.
The gas temperature at the external quartz wall is equal to 300 K. At the inlets (z = 0) the temperature (T = 400K) and the axial velocity of the transporting, central and sheath gases (in corresponding with G₁, G₂ and G₃) are set constant. At the outlet (Z₄=400mm) the pressure is set constant P = Pₘₐₓ = 10⁵ Pa. The boundary conditions for the Maxwell equations are given as in accordance with [10].

In numerical calculations it is set that the transporting, central and sheath gases are Ar–H₂ mixture with a variation of hydrogen volume fraction α = 0–10%. The thermophysical parameters and electrical conductivity of Ar-H₂ plasma are obtained in the approximation of local thermodynamic equilibrium from calculated data [19–21].

The numerical simulation of equations (1) - (8) is based on the finite volume method. The meshes in the calculating zones are built in ANSYS ICEM CFD package using HEXA 8 hexagonal structure blocks.

3. Results and Discussion

The main reason for the arose of a vortex tube in front of the coils zone is because of the formation of high pressure zone [17] near the axis of the plasma torch (Fig. 2), which is domain by the radial component of the electromagnetic force in the plasma. The working gases flow into this zone and form the main (first) toroidal vortex before the coils zone (under certain conditions). The discharge current Jcoil determines the level of magnetic pressure, and, as a result, the level and size of the high pressure zone (Fig. 2). Consequently, it found that there is a critical current Jcr. The value Jcr separates the plasma flow regimes into the potential (Jcoil ≤ Jcr) and vortical regimes (Jcoil ≥ Jcr). A main toroidal vortex will be formed before the coils zone when the discharge current Jcoil exceed the critical value Jcr.

![Figure 2](image_url) The streamlines (colored lines), temperature contour T = 8000 K (dashed lines) and pressure contour ΔP = 6 Pa (solid lines) under Jcoil = 170 A: α=0% – upper half-plane; α=5% – lower half-plane.

As the results in [17], the critical current Jcr =90–100A for argon plasma torch with three coils. The use of Ar-H₂ mixtures as working gas leads to a change of the thermodynamic parameters and flow regimes in the ICP plasma (Fig.2) because of its lower electrical conductivity, higher heat capacity and thermal conductivity [20], compared to pure argon (under the same temperature). In all of those figures the red dots indicate the locations of the inductor coils, and the black lines indicate the walls of the ICP plasmotron.

It is found that under the same discharge current Jcoil the joule heating zone and its volumetric density q are reduced in the Ar–H₂ plasma in comparison to that in the pure argon plasma. As can be seen in Fig. 2, this leads to a decrease of high temperature zone of plasma (the isothermal dashed lines T = 8 kK are reduced) and the maximum plasma temperature. Note that, with an increase of volume fraction α the distribution of temperature in the plasma zone becomes more homogeneous because of the higher thermal conductivity of hydrogen plasma. What's more, the transitions from the potential to vortical regimes are observed at higher discharge current. The dependence of the critical discharge current Jcr on the volume fraction of hydrogen α can be approximated by the linear function Jcr≈ 100 + 10α(%).

The dependencies of the axial coordinate Z of the vortex center on the discharge current (under various α) are shown in Fig. 3 (dashes lines). In pure argon plasma (α = 0) Z is practically located at the cross section of the first coil (Zₐₙₙ=63 mm) when the discharge current Jcoil = Jcr ≈ 100 A. In this case the increase of discharge current Jcoil leads to a monotonous decrease of Z, to the minimum limiting value Zₘᵢₙ ≈ 50 mm (i.e. the vortex center is shifted left to meet the oncoming stream).
For Ar-H₂ plasma, the increase of discharge current \( J_{\text{coil}} \) above the critical value \( J_{\text{cr}} \) will also lead to a decrease of \( Z_v \) to the corresponding minimum limiting values, which coincide with the limiting value \( Z_v, \text{min} \approx 50 \text{ mm} \) in the pure Ar plasma when \( \alpha = 0\% \).

The dependencies of vortex intensity \( \epsilon_v \) of the main vortex tube (before the coils zone) on the discharge current \( J_{\text{coil}} \) are shown in Fig.3 (solid lines). The vortex intensity \( \epsilon_v \) is defined as \([14]\): \( \epsilon_v = G_v/(G_1 + G_2) \), where \( G_v \) is the backflow rate of gas in the vortex zone. In all of the three cases \( \epsilon_v \) is a monotonically increasing function of the discharge current. At significant discharge currents \( J_{\text{coil}} \geq 200-250 \text{ A} \) the intensity of the vortex tube \( \epsilon_v \) becomes more than one unit \( (\epsilon_v > 1) \). This means that part of the sheath gas flow begins to participate into the formation of the main vortex.

![Figure 3](image)

**Figure 3.** The dependencies of the vortex intensity \( \epsilon_v \) (solid lines) and the axial coordinate of the vortex center \( Z_v \) (dashed lines) on the discharge current \( J_{\text{coil}} \) under different volume fraction of hydrogen: 1–\( \alpha = 0\% \); 2–\( \alpha = 5\% \); 3–\( \alpha = 10\% \).

It is investigated that in the vortical regime under the same discharge current \( J_{\text{coil}} \geq J_{\text{cr}} \) the intensity of the main vortex tube in pure Ar plasma \( (\alpha = 0) \) is greater or equal to that in the argon-hydrogen plasma \( (\alpha \neq 0) \). That is, the values of \( \epsilon_v \) and \( Z_v \) under \( \alpha = 0 \) are the upper limits of the \( \epsilon_v(J_{\text{coil}}) \) and \( Z_v(J_{\text{coil}}) \) functions under all other different compositions of Ar–H₂ plasma\( (\alpha \neq 0) \).

In the vortical regime \( (J_{\text{coil}} \geq J_{\text{cr}}) \) an increase of the discharge current may causes the formation of a shedding plasma flow directly behind the coils zone near the quartz wall and, accordingly, a second vortex tube is formed (with the opposite direction of rotation to that of the first vortex) (Fig.4). The second vortex tube arises only after that when the main vortex has formed. So the critical current \( J_{\text{cr}}^* \), at which the second vortex is formed, is higher than \( J_{\text{cr}} \). With the increase of \( \alpha \) in Ar–H₂ plasma, this critical current \( J_{\text{cr}}^* \) becomes closer to \( J_{\text{cr}} \), in particular, for \( \alpha = 10\% \) this critical current value is approximately equal to \( J_{\text{cr}} (J_{\text{cr}}^* \approx J_{\text{cr}} = 200 \text{ A}) \).

The intensity \([22]\) of the second vortex tube can be described using the parameter \( \Gamma_v = \frac{\oint U \, d\ell}{\pi} \) (the integration is carried out along the centerline of vortex cross section), which is a monotonically increasing function of the discharge current. When \( J_{\text{coil}} = 230 \text{ A} \) (at \( \alpha = 10\% \)), its intensity \( \Gamma_v \approx 0.11 \text{ m}^2/\text{s} \) becomes comparable with the intensity of the main vortex tube \( (\Gamma_v \approx 0.34 \text{ m}^2/\text{s}) \). It is found that the presence of a second vortex near the quartz wall may cause some problems such as the heat transfer between the plasma torch and the quartz pipe.
Figure 4. The streamlines (colored lines), temperature contour \( T=8000 \text{ K} \) (solid lines) and pressure contour \( \Delta P = 6 \text{ Pa} \) (solid lines) under \( \alpha=10\%: J_{\text{coil}}=200 \text{ A} \) – upper half-plane; \( J_{\text{coil}}=230 \text{ A} \) – lower half-plane.

4. Conclusions
The thermodynamic parameters and structure of the argon-hydrogen plasma flow pattern in the channel of RF ICP plasma torch are obtained. The features of the distribution of velocity and temperature fields are found in the ICP plasma torch under the presence of toroidal vortex flows. It is established that the necessary condition for the form of main vortex tube is that the discharge current exceeds an critical value \( J_{\text{cr}} \), which depends on the volume fraction of hydrogen \( \alpha \): \( J_{\text{cr}} \approx 100 + 10\alpha(\%\), A. The intensity and position of the main vortex tube in supercritical flow regimes are determined as a function of the discharge current and volume fraction \( \alpha \). It is shown that under the same discharge current, the intensity of the vortex tube in the pure argon flow is greater or equal to \( \varepsilon_{\text{v}} \) in the Ar–H\(_2\) mixture flows (\( \alpha \neq 0 \)).

References
[1] Grishin Yu M, Kozlov N P and Skryabin A S 2012 High Temperature 50 491.
[2] Grishin Yu M, Kozlov N P and Skryabin A S 2016 High Temperature 54 619.
[3] Ryzhkov S V 2011 Plasma Physics Reports 37 1075
[4] Chirkov A Yu, Ryzhkov S V, Anikeev A V and Bagryansky P A 2011 Fusion Science and Technology 59 (1T) 39
[5] Kuzenov V V and Ryzhkov S V 2016 Bulletin of the Russian Academy of Sciences. Physics 80 598
[6] Bibikov M B, Demkin S A, Zhivotov V K, Zaitsev S A, Moskovskii A S, Smirnov R V, Fateev V N 2010 High Energy Chemistry 44 58.
[7] Gonzalez N Y, Morsli M E and Proulx P 2008 Journal of Thermal Spray Technology 17 533.
[8] Sanaz A E 2013 A modeling framework for the synthesis of carbon nanotubes by rf plasma technology (Toronto: University of Toronto).
[9] Ameya B, Christopher R P, Steven A C and Carter C B 2003 J. Appl. Phys. 94 1969.
[10] Colombo V, Ghedini E and Sanibondi P 2010 Plasma Sources Science and Technology 19 65.
[11] Morsli M E and Proulx P 2007 J. Appl. Phys. 40 387.
[12] Ye R B, Proulx P and Boulos M I 1999 International Journal of Heat and Mass Transfer 42 1585.
[13] Grishin Yu M and Miao Long 2017 Journal of Physics: Conf. Series 830 012069.
[14] Punjabi S B, Sahasrabudhe S N, Joshi N K, Mangalvedkar H A, Das A K and Kothari D C 2014 Physics of Plasmas 21 24.
[15] Novikov I N and Kruchinin A M 2014 Technical Physics Letters 40 17.
[16] Cian L J, Lin J Z and Yu M Z 2013 Journal of Thermal Spray Technology 22 1024.
[17] Grishin Yu M and Xiao Long 2016 Applied Physics A 113[3,3][in Russian].
[18] Morozov A I 2008 Introduction to plasma dynamics (Fizmatlit, Moscow) [in Russian].
[19] Murphy A B 2000 Plasma Chemistry and Plasma Processing 20 279.
[20] Boulos M I, Fauchais P and Pfender E 1994 Thermal plasmas: fundamentals and applications, Volume 1 (New York).
[21] Holik E F 2008 Simulation results of an inductively coupled rf plasma torch in two and three dimensions for producing a metal matrix composite for nuclear fuel cladding (m.s. thesis: Texas A&M University).
[22] Bizyaev I S, Borisov A V, Mamaev I S 2016 Regular and chaotic dynamics 21 367.