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Three-dimensional modelling of inductively coupled plasma torches

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Abstract. A three-dimensional model has been developed for simulating the behaviour of inductively coupled plasma torches (ICPTs), using customized CFD commercial code FLUENT©. The helicoidal coil is taken into account in its actual 3-D shape, showing the effects of its non-axisymmetry on the plasma discharge. Steady state, continuity, momentum and energy equations are solved for argon optically thin plasmas under the assumptions of LTE and laminar flow. The electromagnetic field is obtained by solving the 3-D vector potential equation on a grid extending outside the torch region. In order to evaluate the importance of various 3-D effects on calculated plasma temperature and flow fields, comparisons of our new results with the ones obtainable from conventional 2-D models and from an improved 2-D model that includes 3-D coil effects are presented. The presence of wall temperature hot spots due to plasma discharge displacement from the torch axis is evidenced, while the use of the new 3-D code for optimization of induction coil geometry and plasma gas inlet features is foreseen.

PACS. 52.75.Hn Plasma Torches – 52.65.-y Plasma simulation – 52.80.Pi High-frequency and RF discharges

1 Introduction

Inductively coupled plasma torches have been used over the years as an effective tool for producing thermal plasma jets in many different industrial applications, such as atmospheric or soft vacuum plasma spraying for deposition of metals, thermal plasma waste treatment, plasma assisted chemical vapour deposition, plasma preparation of ultra-fine powders, just to mention a few [1]. Together with RF plasma torch evolution in industrial and fundamental science research, in order to gain deep understanding of the physical and chemical processes occurring within these systems, many efforts have been devoted to mathematically modelling the plasma flow and heat transfer coupled with the electromagnetic field [2–7]. Recent work has been devoted to the optimization of steady state and time dependent two-dimensional simulation models [6,7], also extending the calculating domain of the electromagnetic field induced by the idealized axisymmetric induction coil outside of the plasma discharge region and using simplified boundary conditions, both within conventional codes and using the commercial code FLUENT© [5,7–11]. In fact, FLUENT© offers important advantages in the modelling of inductively coupled plasma torches, such as the possibility of studying complicated geometries and easily generating both structured and non-structured meshes. However, by itself, FLUENT©, at the moment, can only solve mass, momentum and energy conservation equations for the plasma, but it does not include a module for electromagnetic field calculations. To overcome this problem one can either add to the FLUENT© solver two new User-Defined Scalars (UDS) for the real and imaginary parts of the complex vector potential (UDS approach) [8] or develop a C User-Defined Function (UDF) which fully solves the vector potential equation, while letting the commercial code solver compute only the plasma temperature and velocity fields (UDF approach) [9]. A novel two-dimensional FLUENT© based model to calculate the electromagnetic fields in inductively coupled plasma torches, has been recently developed [10,11], showing that some three-dimensional effects arise when the inclined angle of current in an idealized concentric cylinder coil is kept into account: influences on plasma flow and temperature are negligible, but the plasma shows some swirling effects due to Lorentz forces induced by the axial electric field and radial magnetic field. Mathematical modelling of 3-D mixing for the downstream region of an inductively coupled plasma torch has been also proposed, but only for a computational domain that did not include the induction coil [12]. In this paper we briefly sketch a novel three-dimensional model where the helicoidal coil is taken into account in its actual 3-D shape, showing the effects of its non-axisymmetry on the plasma discharge.

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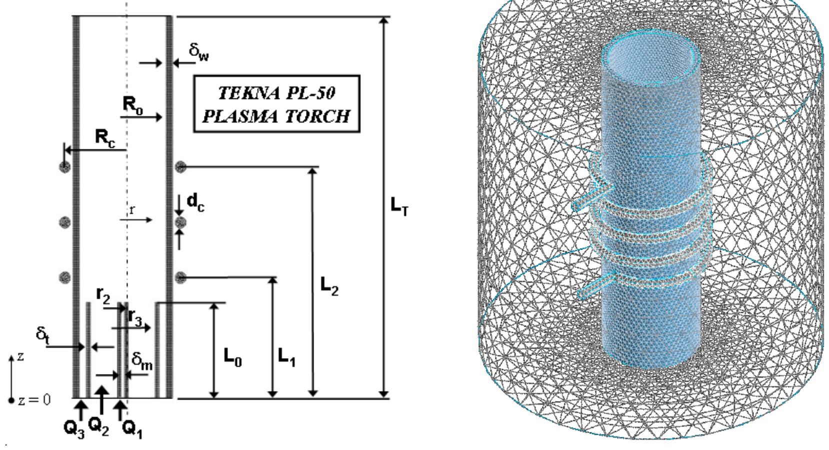


(a) (b)

Fig. 1. (a) Torch geometry and operating conditions; (b) schematic of the extended-field electromagnetic model grid, where vanishing vector potential boundary conditions are set at a distance of 0.1 m from the torch axis and on planes $z = 0$ and $z = 0.2$ m. $L_0 = 50$ mm, $L_1 = 60$ mm, $L_2 = 124$ mm, $L_T = 200$ mm, $r_2 = 3.7$ mm, $r_3 = 18.8$ mm, $R_0 = 25$ mm; $R_c = 33$ mm, $\delta_m = 2.0$ mm, $\delta_t = 2.2$ mm, $\delta_W = 3.5$ mm, $d_c = 6$ mm, $Q_1 = 1$ slpm, $Q_2 = 3$ slpm, $Q_3 = 31$ slpm, $P = 5$ kW, $f = 3$ MHz.

Within this paper, the effect of the electrostatic potential due to accumulated charge in the plasma has not been kept into account; it can be quite safely foreseen that its effect on plasma behaviour will be mainly limited to slightly changing swirl velocity, while it will not significantly effect plasma temperature distribution. A brief selection of results shows that important effects besides the existence of a swirl velocity occur in the plasma within a 3-D approach: mainly, depending on induction coil geometry (coil length in z-direction, inclination of coil turns, shape of coil ending sections), a displacement of the plasma fireball from the torch axis can be evidenced, together with hot spot formation for the temperature of the plasma containment tube; the amount of this displacement increases with increasing non-axisymmetry of coil geometry. Based on these results, the impact of the new model on design, optimization and diagnostics of inductively coupled plasma torches might be of some interest. In this paper the first abovementioned approach for using FLUENT© has been followed; due to the increase of computation effort for 3-D cases, the need for improvements on the electromagnetic model and on the definition of the computational domain and related boundary conditions, as already performed by the authors for 2-D cases [9], can be foreseen, using a FLUENT© linked external routine that allows a limitation of the fluid-dynamic domain to the torch region. The code has been tested against literature results obtained with 2-D models [8,9] and with 2-D models with 3-D effects [10,11]. Within the new 3-D model, the effect on plasma flow and temperature fields of changing electric and operating conditions in inductively coupled plasma torches still need to be investigated and will not be part of this work.

2 Modelling approach

The fluid-dynamic model of the torch includes the 3-D continuity, Navier-Stokes and energy equations for the optically thin argon plasma, under the assumptions of laminar flow and LTE conditions. For the sake of brevity, we do not give all the model details here, since they can be obtained by simply extending the 2-D flow field equations presented in [7] to a 3-D configuration. The electromagnetic field equations are solved together with the fluid-dynamic ones by means of the FLUENT© code, using the extended grid model with vanishing boundary conditions (see Fig. 1b) within the UDS approach, as done in [8–11] for a 2-D domain. A 3-D Cartesian orthogonal (x, y, z) system of coordinates is adopted for the calculations and the induction coil is accurately modelled in its 3-D actual shape, using non-structured meshes (number of meshes used in the calculations; coil: $\sim 8.5 \times 10^3$; electromagnetic field for the region extending outside the torch: $\sim 10^5$; plasma region: $\sim 3.5 \times 10^5$). The governing equations for the three Cartesian components of the vector potential $\mathbf{A} = (A_x, A_y, A_z)$ and for the electric scalar potential, V, can be written as:

$$\nabla^2 \mathbf{A} - \mu_0 \varepsilon_0 \frac{\partial^2 \mathbf{A}}{\partial t^2} = -\mu_0 \mathbf{J} \quad (1)$$

$$\nabla^2 V - \mu_0 \varepsilon_0 \frac{\partial^2 V}{\partial t^2} = -\frac{\rho}{\varepsilon_0} \quad (2)$$

where ε_0 and μ_0 are the dielectric constant and the permeability of the free space, respectively, ρ is the electric charge density in the plasma and $(-\mu_0 \varepsilon_0 \partial^2 \mathbf{A}/\partial t^2)$ accounts for the displacement current associated with the oscillatory magnetic field. The total electric current

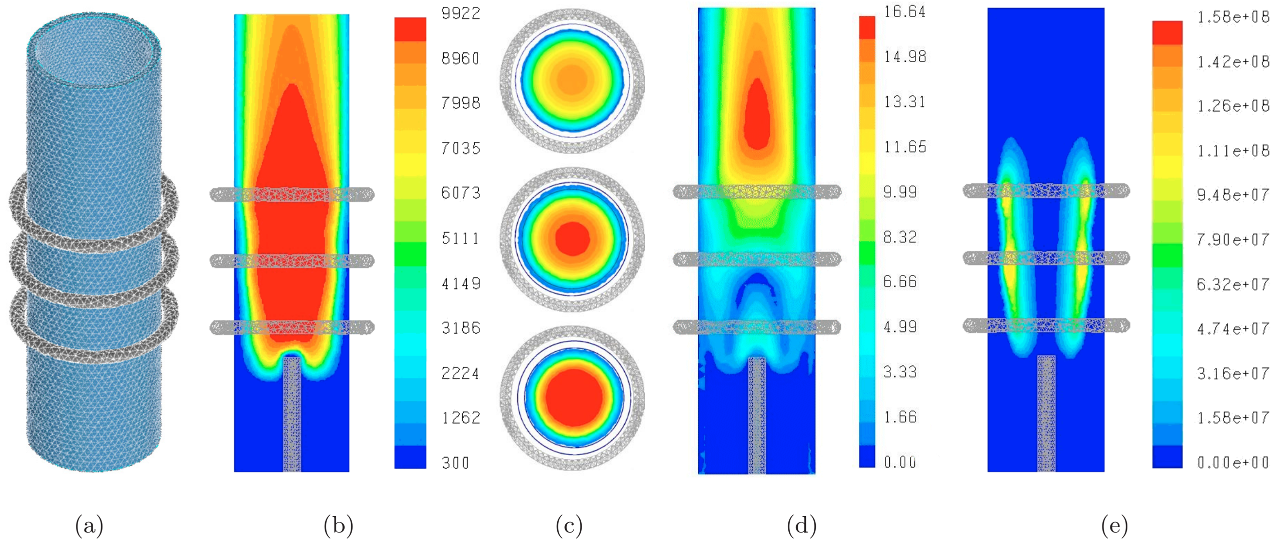


Fig. 2. *CASE I: axisymmetric ring-shaped coil.* (a) Schematic of the plasma confinement tube and induction coil; (b) plasma temperature [K], (d) plasma velocity magnitude [m/s] and (e) power dissipation in the plasma [W/m^3] on a vertical plane passing through the axis of the torch. (c) Temperature distributions in the plasma and wall regions on horizontal planes located at different height in the torch: $z = 0.1$ m, $z = 0.15$ m and $z = 0.2$ m, respectively, from bottom to top.

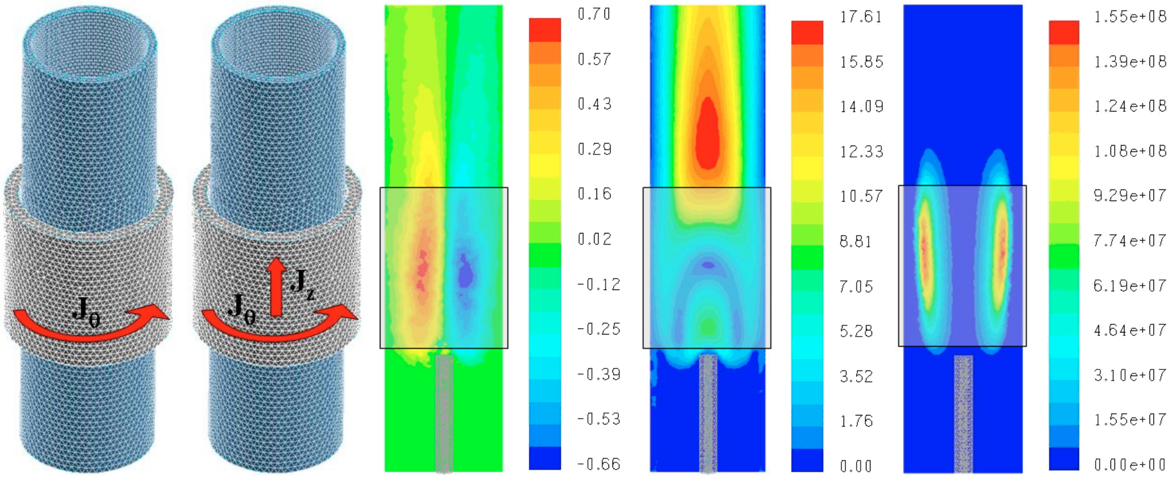
density, $\mathbf{J}$, is given by: $\mathbf{J} = \sigma\mathbf{E} + \mathbf{J}^{(\mathrm{coil})}$, being $\sigma\mathbf{E}$ (where σ is the plasma electric conductivity) and $\mathbf{J}^{(\mathrm{coil})} = (J_x^{(\mathrm{coil})}, J_y^{(\mathrm{coil})}, J_z^{(\mathrm{coil})})$ the current densities in the plasma and in the coil, respectively, while the electric charge density, ρ, is computed by means of the continuity equation: $\boldsymbol{\nabla} \cdot \mathbf{J} = -\partial\rho/\partial t$. In the present model, $\mathbf{J}^{(\mathrm{coil})}$ is calculated as: $\mathbf{J}^{(\mathrm{coil})} = (I/S_c)\mathbf{j}_{\mathrm{coil}}$, where I is the electric current flowing through the coil, and $\mathbf{j}_{\mathrm{coil}}$ is a unit vector perpendicular to the cross-sections of the coil, being S_c the area of these cross-sections for either each coil turn or for the axisymmetric cylindrical coil. In the calculations carried out in this work, the value of I is updated during the calculation process, in order to keep constant the net power dissipated in the plasma. The electric field $\mathbf{E} = (E_x, E_y, E_z)$ and the magnetic field $\mathbf{B} = (B_x, B_y, B_z)$ can be expressed through the definitions of the vector and scalar potentials:

$$\mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} - \boldsymbol{\nabla} V; \quad \mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}.$$

By assuming that $\mathbf{A}$, V, $\mathbf{J}$, ρ, $\mathbf{E}$, $\mathbf{B}$ are all sinusoidal in time with the same frequency f, the standard phasor notation can be used to solve equations (1, 2). All the calculations have been performed by supposing negligible the effect of the scalar potential and of the displacement current associated with the oscillatory magnetic field on flow and temperature fields, solving only a simplified version of equation (1). The former assumption seems to be reasonable since the axial component of the current density in the plasma, which generates a non-uniform electric charge density distribution, is of lower order of magnitude compared to the component on the (x, y)-plane. Preliminary calculations carried out by solving both equations (1, 2) without any simplifications seem to indicate that minor changes in the plasma temperature distribution are to be expected when taking into account also the scalar potential effect, although the plasma swirl velocity might be slightly influenced by the additional contribution to the Lorentz force. However, as these results are part of a work which is still in progress, they will be published in a future, more comprehensive paper.

3 Test-cases and selected results

The torch geometry (PL-50 – Tekna Plasma Systems Inc.), dimensions and axially injected gas flow rates are sketched in Figure 1a and all results will refer to the same total axial length ($L_2 - L_1$, in Fig. 1a) of the coil region but for different coil configurations; the argon plasma is simulated at atmospheric pressure, while the RF generator frequency and the net power dissipated in the plasma are set at 3 MHz and at 5 kW, respectively. In Figure 2 a test-case (CASE I) with an axisymmetric ring-shaped coil is considered; results obtained with the 3-D code for temperature, velocity magnitude and power dissipation in the plasma show a full agreement with literature results [8,9]. Temperature distributions in the plasma and in the containment wall regions on horizontal planes located at different height in the torch are also shown. Some other test-case results (CASE II and III) are presented in Figure 3, where two axisymmetric cylindrical coil configurations are taken into account, with only a tangential current and under the conditions of a 3.7° inclined angle for coil current, respectively, as done under different torch operating conditions in [10,11]. Once again, the 3-D code shows results in agreement with what should be expected taking into account recent 2-D results [10,11] for plasma velocity



(a) (b) (c) (d) (e)

Fig. 3. *CASE II-III: axisymmetric cylindrical coil.* Schematic of the plasma confinement tube and induction coil in the cases of (a) tangential current and (b) tangential and axial current; on a vertical plane passing through the axis of the torch: (c) orthogonal component of swirl velocity [m/s] for case (b) ⊗⊙; (d) plasma velocity magnitude [m/s] and (e) power dissipation in the plasma [W/m^3], for both case (a) and (b). The temperature field for (a) and (b) is very close to the one shown in Figure 2b.

magnitude, power dissipation in the plasma and plasma swirl velocity caused by swirling Lorentz forces. Temperature field for the coil configurations of Figures 3a and 3b is very close to the one of Figure 2b and, therefore, it is not presented. A full exploration of the grid dependency of the numerical results when changing torch geometry and operating conditions has been here omitted. A brief selection of results obtained by means of the new 3-D code for non-axisymmetric coil configurations is presented in Figures 4 and 5 (CASE IV and V), dealing with a 3.5 turns induction coil with inclination 4.73° and with a 5 turns one with inclination 3.68°, respectively. Due to the limited amount of space, in this paper only results (plasma temperature, plasma velocity magnitude, orthogonal component of plasma swirl velocity, distribution of power dissipation in the plasma, orthogonal component of Lorentz forces, real part of the orthogonal component of vector potential) on two planes passing through the axis of the torch and whose relative position is evidenced by coil view will be presented, together with temperature distributions in the plasma and wall regions on horizontal planes located at different height in the torch. While in references [10,11] it is demonstrated that no relevant effect on plasma temperature is induced by taking into account an inclined coil current, different degrees of displacement of the plasma temperature distribution from the torch axis, depending on coil geometry, are now evidenced in Figures 4b and 5b. This effect is strongly related to the non-axisymmetry of plane perpendicular Lorentz forces as evidenced in Figure 5f by a 3-D modelling of the electromagnetic field and it has been observed in some ICPTs with air-cooled quartz tube, together with unstable behaviour of the plasma in the discharge region depending on operating conditions and plasma stabilization mechanism [5,13,14]. Figures 4c and 5c put into evidence the formation of hot spots for the temperature of the torch wall and this result might be validated through future experimental work in various torch operating conditions. As already evidenced in [10,11], the swirling Lorenz forces cause some relevant plasma swirling, as shown by Figures 4d and 5d. For CASE V also some selected results concerning the distribution of power dissipation in the plasma (Fig. 5e) and the real part of vector potential (Fig. 5g) are presented. Negative values in Figures 3c, 4d, 5d, 5f and 5g arise as FLUENT© output due to the use of a 3-D Cartesian orthogonal (x, y, z) system of coordinates, while the slight non-axisymmetry of results for the orthogonal component of swirl velocity in Figure 3c is due the non-axisymmetry of the 3-D computational grid inside the torch and is to be considered as a mere numerical effect. While a future, more comprehensive study, will show in detail also the effect on the discharge of non uniform charge distribution in the plasma, this brief selection of results for the newly developed three-dimensional code is sufficient to show its significance in the prediction of phenomena at present still neglected in the simulation of inductively coupled plasma torches.

4 Conclusions and future developments

In this paper a new three-dimensional model has been presented for the realistic investigation of the behaviour of inductively coupled plasma torches for different induction coil geometries and for fixed operating conditions, using the commercial code FLUENT©. The new code has been validated against test-case literature results [8,9] for 2-D axisymmetric torch configurations and against recent 2-D

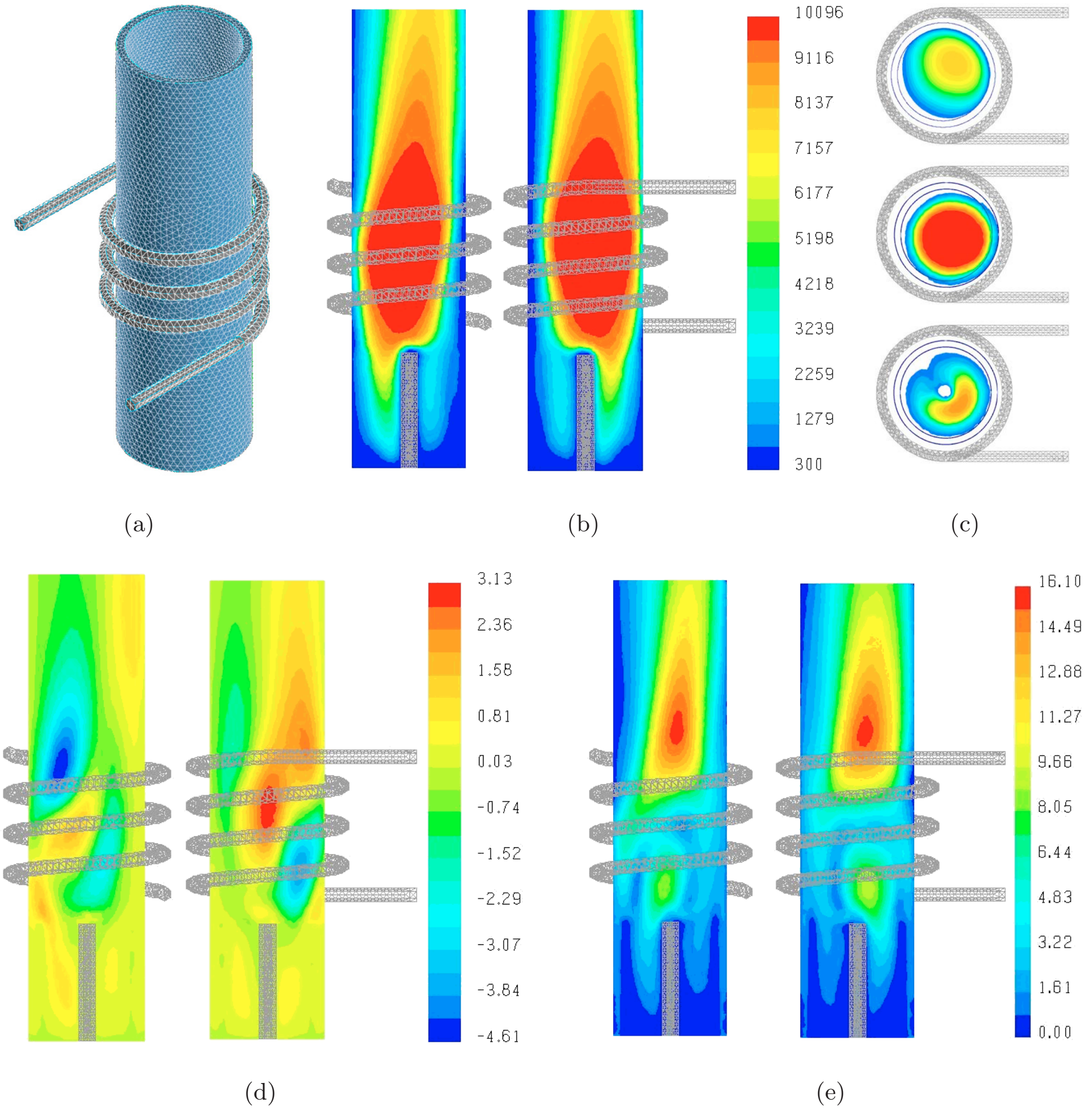


Fig. 4. *CASE IV: 3.5 turns with coil inclination 4.73°.* (a) Schematic of the plasma confinement tube and induction coil; on two planes passing through the axis of the torch, whose relative position is evidenced by coil view: (b) plasma temperature fields [K], (d) orthogonal component of swirl velocity [m/s] ⊗⊙, (e) plasma velocity magnitude [m/s]; (c) plasma and wall temperature fields [K] on three horizontal planes located at different height in the torch: $z = 0.05$ m, $z = 0.1$ m, $z = 0.2$ m, respectively, from bottom to top.

results [10,11] that show some 3-D effects induced by a more realistic description of coil current. Our 3-D results confirm that negligible effects on plasma temperature distribution arise when only the axial component of induction coil current is taken into account within an axisymmetric coil configuration [10,11], while most important effects on non-axisymmetry of such distribution are evident when the real induction coil shape is considered. Some selected results have been presented, showing different degrees of displacement of the plasma fireball from the torch axis, depending on coil geometry and, as a consequence, the formation of hot spots for the temperature of the torch wall. The effect of keeping into account the electrostatic potential generated by charge accumulation in the plasma has been here neglected, while it will be fully considered in a future work, which will also show, for each torch and coil geometry, the relative importance of 3-D effects when changing torch operating conditions (discharge power, gas flow rates) for a wide range of induction coil configurations; anyway, preliminary results [15] let us foresee that a modelling approach that includes the electrostatic potential induces no main effect on plasma fireball displacement, while swirl velocities in the plasma slightly increase. Improvements on the electromagnetic model treatment, already performed by the authors in [9] for 2-D cases, together with grid and computation domain optimization,

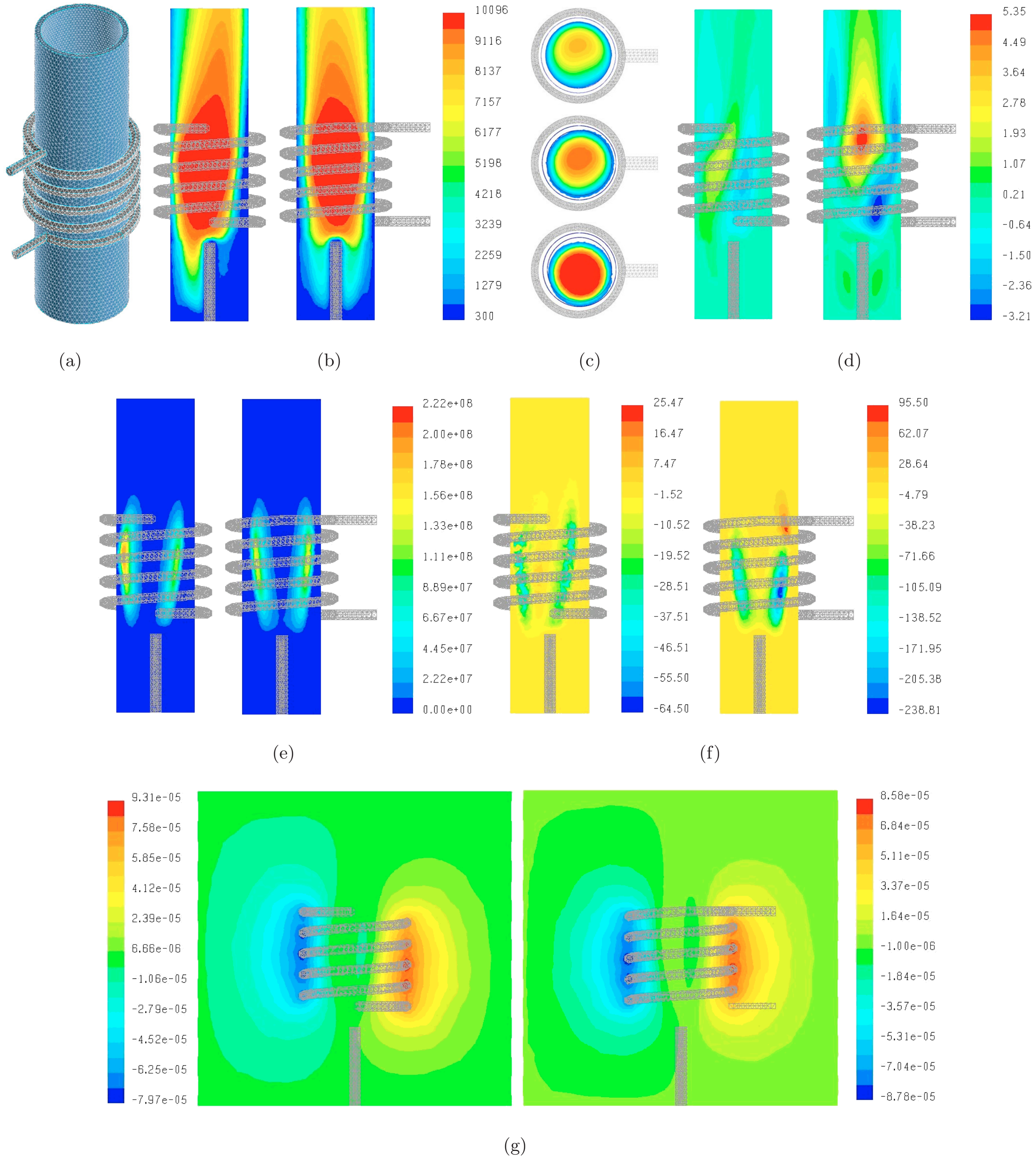


Fig. 5. *CASE V: 5 turns with coil inclination 3.68°*. (a) Schematic of the plasma confinement tube and induction coil; on two planes passing through the axis of the torch, whose relative position is evidenced by coil view: (b) plasma temperature [K], (d) orthogonal component of swirl velocity [m/s] ⊗⊙, (e) power dissipation in the plasma [W/m^3], (f) orthogonal component of Lorentz force [N/m^3] ⊗⊙ and (g) real part of the orthogonal component of the vector potential [T m] ⊗⊙; (c) temperature distributions in the plasma and wall regions on horizontal planes located at different height in the torch: $z = 0.1$ m, $z = 0.15$ m and $z = 0.2$ m, respectively, from bottom to top.

need to be exploited in the future also for 3-D modelling, using a linked external routine that allows a limitation of the fluid-dynamic domain to the torch region. The newly developed code let us also foresee the possibility of showing the real effects of the system non-axisymmetry of the temperature distribution on trajectories of particles injected in the plasma and opens the field for optimization of coil geometry and torch operating conditions.

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