Large-Eddy Simulation of Subsonic-Supersonic Flow and Heat Transfer in a Hybrid Gas–Water Stabilized Arc

J Jeništa\(^1\), H Takana\(^2\), H Nishiyama\(^2\), M Bartlová\(^3\), V Aubrecht\(^3\) and P Křenek\(^1\)
\(^1\)Institute of Plasma Physics AS CR, v.v.i., Za Slovankou 3, 182 00 Praha 8, Czech Republic
\(^2\)Institute of Fluid Science, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai, Miyagi, 980-8577, Japan
\(^3\)Brno University of Technology, Technická 8, 616 00 Brno, Czech Republic

E-mail: jenista@ipp.cas.cz

Abstract. The paper presents numerical simulations of the turbulence effect in the discharge and near-outlet regions of the hybrid-stabilized argon-water electric arc. Calculations were carried out for the assumption of laminar and turbulent plasma flow models, respectively. Results of simulation for currents 300-600 A on a fine numerical grid show that the influence of turbulence is weak and the maximum difference for all the monitored physical quantities is less than 2% in the discharge region and less than 6% in the near-outlet region. Comparison with experimental temperature profiles exhibits good agreement.

1. Introduction
The so-called hybrid-stabilized electric arc, which was developed a decade ago at the Institute of Plasma Physics AS CR, v.v.i. (IPP AS CR, v.v.i.) in Prague, utilizes a combination of gas and vortex stabilization. A picture and its principle is shown in figure 1. In the hybrid argon–water plasma torch, the arc chamber is divided into the short cathode part, where the arc is stabilized by tangential argon flow, and the longer part, stabilized by water vortex created by tangential injection of water in the chamber. The arc burns between the cathode, made of a small piece of zirconium pressed into a copper rod, and the external water-cooled rotating disc anode, made of a copper and placed a few millimeters downstream of the torch nozzle exit. This arrangement provides not only the additional stabilization of the arc in the cathode region and the protection of the cathode tip, but also offers the possibility of controlling argon–water plasma jet characteristics in a wider range than that of pure gas- or liquid-stabilized arcs [1]. The experiments made on this type of torch [2] showed that the plasma mass flow rate, velocity and momentum flux in the jet can be controlled by changing the mass flow rate in the gas-stabilized section, whereas thermal characteristics are determined by the processes in the water-stabilized section.

The hybrid arc has been used at IPP AS CR, v.v.i., in the plasma spraying torch WSP®H (160 kW) for spraying metallic or ceramic powders (TiO\(_2\), Al\(_2\)O\(_3\), ZrSiO\(_4\), W-based, Ni-based alloys, Al, steel) injected into the plasma jet [3]. Several years ago, an experimental plasmachemical reactor PLASGAS equipped with the spraying torch WSP®H was utilized for the innovative and environmentally friendly plasma gasification and pyrolysis of wastes with a perspective to their sustainable energetic and chemical valorization and to a reduction of the emission of greenhouse gases [4]. Pyrolysis of biomass
was experimentally studied in a reactor using crushed wood, sunflower seeds or rubber oil as model substances. A high content of a combustible mixture of hydrogen and carbon monoxide was produced (i.e., syngas).

Some of our previous calculations analyzed flow regimes, thermal, electrical characteristics and power losses from the hybrid-stabilized electric arc [5-6]. Images of plasma jet taken with the fast shutter camera show the laminar structure of the plasma flowing out of the discharge chamber downstream of the nozzle exit for currents up to 600 A, i.e., the operational regime of our torch. Our previous calculation demonstrates that the Reynolds number based on the 6 mm outlet diameter reaches 13,000 at maximum in the axial region just behind the exit nozzle and decreases to 300 in arc fringes.

The type of flow inside the discharge chamber has been already studied in [7] and it was concluded that the influence of turbulence inside the discharge region is small. Here we study this phenomenon in more detail. First, since the difference between laminar and turbulent flow regimes is expected to be small, it is necessary to adjust numerical grid to reduce at the minimum grid-dependence of the calculated physical quantities. Second, the character of flow was investigated here not only inside the discharge region as in [7] but also in the nozzle and near-outlet regions of the arc torch.

Sections 2 and 3 provide information about the model assumptions, plasma properties, boundary conditions and the numerical scheme. Section 4 reveals the most important findings and a comparison of our calculated results with experiments.

![Figure 1: The plasma spraying torch WSP®H with hybrid stabilization (left), i.e., the combined stabilization of the arc by axial gas flow (Ar or N\textsubscript{2}) and water vortex. The principle of the hybrid plasma torch WSP®H is shown at right. The calculation domain is shown by a red-dashed line.](image)

2. Physical model
The following assumptions for the model were applied:

1) The numerical model is two-dimensional with the discharge axis being the axis of symmetry (axisymmetric);
2) Plasma flow is laminar/turbulent and compressible in the state of local thermodynamic equilibrium (LTE);
3) Argon and water create a uniform mixture in the arc chamber (single gas phase);
4) Only a self-generated magnetic field by the arc itself is considered;
5) Gravity effects are negligible;
6) The partial characteristics method for radiation losses from the arc is employed.

The complete set of conservation equations representing the mass, electric charge, momentum and energy transport of such plasma can be written in the vector notation as follows:

\[ \frac{\partial}{\partial t} \rho + \nabla \cdot (\rho \vec{u}) = 0 \]  

(1)
momentum equations:

\[
\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \mathbf{\tau} + \mathbf{j} \times \mathbf{B},
\]

\[
\tau_{ij} = \eta \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_l} \right), \tag{2}
\]

energy equation:

\[
\frac{\partial e}{\partial t} + \nabla \cdot [(e + p) \mathbf{u} - \lambda \nabla T] = \mathbf{j} \cdot \mathbf{E} + \Phi_{\text{diss}} - \dot{R},
\]

\[
\dot{R} = \dot{E}, \tag{3}
\]

charge continuity equation:

\[
\nabla \cdot (\sigma \nabla \Phi) = 0, \tag{4}
\]

equation of state:

\[
p = \rho R_g (p, T) T. \tag{5}
\]

Here \(\rho\) is the mass density, \(\mathbf{u}\) the velocity vector containing the axial \((u)\) and radial \((v)\) velocity components, \(p\) the pressure, \(\mathbf{\tau}\) the stress tensor, \(\mathbf{j}\) the current density, \(\mathbf{B}\) the magnetic field, \(e\) the density of internal and kinetic energy produced or dissipated in the unit volume, \(T\) the temperature, \(\mathbf{E}\) the electric field strength, \(\Phi_{\text{diss}}\) the viscous dissipation term, \(\dot{R}\) the divergence of radiation flux, \(\Phi\) the electric potential, \(\lambda\) and \(\sigma\) are the thermal and electrical conductivities, respectively, and \(R_g\) is the specific gas constant dependent on pressure and temperature.

The assumption 3 means that argon- and water-plasma species create single gas (or plasma) phase with a constant argon molar fraction everywhere in the discharge. For example, for 500 A and 40 slm of argon, the argon molar fraction in the water-argon plasma is 43\%. No species conservation equation is thus needed to be solved. In the simulation, the appropriate tables of the transport and thermodynamic properties for this argon molar content must be loaded. We have used the set of tables with the argon molar fraction from 0 to 1 with the step of 0.05. The thermodynamic properties and the transport coefficients of the argon-water plasma mixture were calculated according to the Chapman–Enskog method in the 4th approximation [8] for temperatures of 400–50,000 K [9] and pressures of 0.1-0.3 MPa in the local thermodynamic equilibrium. For the temperature range 400 – 20,000 K the total number of 35 chemical species was considered [9]. The calculations of plasma composition were performed using the modified Newton method for the solution of the nonlinear equations system, which is composed of equations of Saha and mass action law type expressing individual complex components by means of basic ones (e, H, O, Ar). The system was completed by the usual particle and charge balance assuming quasineutrality and equilibrium. The use of perfect gas law in the present model (equation of state) is justified by the fact that the Debye–Hückel pressure correction at the given thermodynamic conditions was found to be of the order 10⁻³ which cannot influence the relations between molar fractions [9].

Turbulence was modeled by Large-Eddy Simulation using the Smagorinsky sub-grid scale model [10-13] with the constant values of the Smagorinsky coefficient \((C_s = 0.1)\) and the turbulent Prandtl number \((Pr_t = 0.9)\). To suppress turbulence near the walls, we applied a Van Driest damping function near the walls [10] in the form

\[
l_S = C_S \Delta \left[ 1 - \exp \left( -y^+ / A^+ \right) \right], \tag{6}
\]

where \(l_s\) is the Smagorinsky lengthscale, \(C_s\) is the Smagorinsky coefficient, \(\Delta\) is the filter width, \(y^+\) is the distance from the wall normalized by the viscous lengthscale, and \(A^+ = 25\). The eddy viscosity \(\mu_t\) and the turbulent thermal conductivity \(\lambda_t\) are modeled as [10, 11].
$$\bar{S} = (C_{S}\Delta)^2 S \quad , \quad \lambda_t = c_p \mu_t / P_{r_t} \quad ,$$  \hspace{1cm} (7)

$\bar{S}$ is the characteristic filtered rate of strain and $c_p$ is the specific heat at constant pressure. The filter width $\Delta$ is proportional to the grid size with generally nonequidistant spacing $\Delta x_i$ and $\Delta y_j$, defined here as $\Delta = \Delta_k = \sqrt{\Delta x_i\Delta y_j}$.

Radiation losses from the argon-water arc were calculated by the partial characteristics method for different molar fractions of argon and water plasma species as a function of temperature and pressure. The principle of the method is that the calculation of integrals over radiation frequencies in equations for radiation quantities is performed in advance to form functions $S_{om}$ and $S_{im}$, called partial characteristics \[14\] which include all time demanding integrations over frequencies. These functions are stored in data tables according to several parameters, such as plasma pressure, temperature and geometrical dimensions. The tables are then used in numerical simulations of plasma flow with spatial integrations only. The advantage of this method is that it directly calculates the reabsorption of radiation in the low-temperature regions of the arc. Continuous radiation due to photo-recombination and "bremsstrahlung" processes, discrete radiation consisting of thousands of spectral lines, molecular bands of $O_2$, $H_2$, OH and $H_2O$ have been included in the calculation of partial characteristics \[15\]. Broadening mechanisms of atomic and ionic spectral lines due to Doppler, resonance and Stark effects have been considered.

3. Boundary conditions and the numerical method

The calculation region and the corresponding boundary conditions are presented in figure 2. This configuration agrees with the hybrid torch experimental setup. The only difference in boundary conditions between the laminar and turbulent models is a Van Driest damping function, which is applied only in the turbulent model.

(a) Inlet boundary (AB) is represented by the nozzle exit for argon. Along this boundary we assume the zero radial velocity component, $v = 0$. Because of the lack of experimental data, the temperature profile $T(r, z = 0)$ and the electric field strength $E_z = -\partial \Phi / \partial z = \text{const.}$ for a given current are calculated at this boundary before the start of the fluid-dynamic calculation itself iteratively from the Elenbaas-Heller equation including the radiation losses from the arc. The inlet velocity profile $u(r)$ for argon plasma for the obtained temperature profile $T(r, z = 0)$ is pre-calculated from the axial momentum equation under the assumption of a fully developed flow.

(b) Axis of symmetry (BC). The zero radial velocity and symmetry conditions for the temperature, axial velocity and electric potential are specified here, i.e., $\partial T / \partial r = \partial u / \partial r = \partial \Phi / \partial r = 0$, $v = 0$.

(c) Arc gas outlet plane (CD). The zero electric potential $\Phi = 0$ (the reference value) and zero axial derivatives of the temperature and velocity components are defined at CD, i.e., $\partial T / \partial z = \partial u / \partial z = \partial v / \partial z = 0$.

(d) Arc gas outlet plane (DE). The zero radial derivatives of the temperature, velocity and electric potential are defined here, $\partial T / \partial r = \partial u / \partial r = \partial v / \partial r = \partial \Phi / \partial r = 0$. The total pressure is fixed at 1 atmosphere, $p = 1 \text{ atm}$.

(e) Outlet wall and the nozzle (EF). We specify no slip conditions for velocities, $u = v = 0$, constant values of $E_r$ and $E_z$ ($\partial \Phi / \partial z = \partial \Phi / \partial r = 0$) and $T(r, z) = 773 \text{ K (500° C)}$ for the temperature of the nozzle.

(f) Water vapor boundary (FA). Along this line we specify the so-called “effective water vapor boundary,” designated in Fig. 2 as the “water vapor boundary” with a prescribed temperature of water vapor $T(R = 3.3 \text{ mm}, z) = 773 \text{ K}$. This is a numerical simplification of a more complex physical reality assumed to be near the phase transition water-vapor in the discharge chamber. Since we are not
able to see inside the discharge chamber, the shape of the phase transition between water and vapor in the discharge chamber is not experimentally known and it is unclear as yet if the structure of the transition is simple or very complicated, for example, with a time-dependent form. In Ref. [16] the iteration procedure for determination of the mass flow rate \( \dot{m} \) and the radius of the “water vapor boundary” for each current was proposed. The final corresponding values of water mass flow rates \( \dot{m} \) are: 0.228 g s\(^{-1}\) (300 A), 0.315 g s\(^{-1}\) (400 A), 0.329 g s\(^{-1}\) (500 A), 0.363 g s\(^{-1}\) (600 A). The magnitude of the radial inflow velocity is calculated from the definition of mass flow rate

\[
v(R) = \frac{\dot{m}}{2\pi R \sum \rho(R,z) \Delta z},
\]

where, \( \rho(R,z) \) is a function of pressure and thus dependent on the axial position \( z \), \( \Delta z \) being the distance between the neighboring grid points.

Due to practically zero current density in the cold vapor region (no current goes outside of the lateral domain edges), the radial component of the electric field strength is put at zero, i.e., \( E_r = -\frac{\partial \Phi}{\partial r} = 0 \). The axial velocity component is set to zero, \( u = 0 \).

LU-SGS (Lower-Upper Symmetric Gauss-Seidel) algorithm [17], belonging to the group of the density-based methods coupled with the Newtonian iteration method, are used for the integration of discretized Eqs. (1)–(4) in time and space. To resolve compressible phenomena accurately, the Roe Flux Differential Scheme coupled with the third-order MUSCL-type (Monotone Upstream-centered Schemes for Conservation Laws) TVD (Total Variation Diminishing) scheme are used for a convective term. The electric potential from equation (4) is solved in a separate subroutine by the TDMA (Tri-Diagonal Matrix Algorithm) line-by-line method, including the block correction technique to speed up the convergence. Under-relaxation is employed to avoid divergence.

The computer program was written in the Fortran language. The task was solved on oblique structured grids with nonequidistant spacing. We chose three different grids in order to make numerical tests on grid-independence and appropriate resolution of the LES model. The coarsest grid contains totally 38,553 grid points (Grid1) with 543 and 71 points in the axial and radial directions respectively. The two finer grids have 115,018 (Grid2) and 193,914 (Grid3) grid points with 878 x 131 (Grid2) and 1134 x 171 (Grid3) points in the axial and radial directions respectively.

Figure 2: Discharge area geometry. The origin of the \( r-z \) coordinate system is set at the point B. The dimensions of the domain are 3.3 mm for the radius of the discharge region (AB), 20 mm for the outlet region (Z\(_i\)) and 78.32 mm for the total length (BC). Inlet boundary (AB) is represented by the nozzle exit for argon. Along the line FE the outlet nozzle and the wall of the torch equipment is specified.

4. Results of Calculation

Calculations for the assumptions of turbulent and laminar flows have been carried out for currents 300, 400, 500 and 600 A. The mass flow rate for the water-stabilized section of the discharge was taken for
each current between 300 and 600 A from our previously published work [16]. The values of argon mass flow rates were chosen 22.5, 27.5, 32.5 and 40 slm (standard liters per minute) in accordance with experimental conditions. It was found from the mass and energy balances at the torch exit nozzle [18] that part of argon is taken away before it reaches the torch exit because argon is mixed with vapor steam and removed to the water system of the torch. The amount of argon transferred in such a way from the discharge is around 50% for the currents studied [18]. Since the present model does not treat the mechanism of argon removal in the model, we consider in the calculations that argon mass flow rate present in the discharge equals one-half of argon mass flow rate at the torch inlet (i.e., for 22.5 slm we take 50% of this amount, etc.).

4.1 Grid-independence study

It is known that a computational grid density can influence the stability of a solution, convergence of a solution and the final distribution of physical quantities. It usually holds that an increasing number of grid points changes the distribution of calculated quantities. There is however a limit number of points behind of which the results become nearly independent of the grid density. Here we employed Grids1-3 mentioned above to study this phenomenon.

Some of the results presented in this paper are evaluated as an average quantity in the discharge region or in the nozzle and near-outlet regions. For this purpose we defined two subdomains in the calculation domain - Domain1 and Domain2, displayed in figure 3. Textured Domain 1 includes the whole discharge region and the cylindrical outer region 2 mm thick and 3.3 mm in radius. The yellow Domain2 covers the nozzle wall region and a shear layer between hot plasma and cold surrounding gas with the axial coordinates from 50 to 78 mm and the radial ones between 0 and 5 mm.

Figure 3. Detail of subdomains (Domain1, Domain2) in the whole calculation domain.

Figure 4 shows the relative difference of solutions between two sets of grids – Grid1 and Grid2 (left) and Grid2 and Grid3 (right). Temperature, Velocity and the Mach number are taken at the axial position 2 mm downstream of the nozzle exit, overpressure and the electric potential are taken within the length of the discharge, 0-78 mm (see figure 2). It is obvious that the difference becomes the smallest for the case of finer grids, Grid2 and Grid3, nevertheless the difference even for coarser Grid1 and Grid2 is in this case less than only 0.6%. The same tendency occurs for all studied currents and mass flow rates.

Figure 5 presents the so called space-average relative difference between turbulent and laminar models in Domain1 and Domain2 (see figure 3) for velocity, Reynolds number and temperature. The space-average relative difference for a given physical quantity $X$ is calculated as
where $N$ is the total number of grid points in Domain1 or Domain2; “turb” and “lam” stand for the turbulent and laminar values of $X$, respectively. Grid density is defined as the ratio of the number of grid points to the Grid1 number of points (Grid2 ~ grid density = 3, Grid3 ~ grid density = 5). The results shown here demonstrate that, except for temperature, the space-average relative difference is higher in Domain2 due to the increased eddy viscosity in the shear layer (a transition region between the hot arc and the surrounding atmosphere with steep radial gradients). The maximum difference reaches several per cent. One can also see that space-average relative differences for Grid2 and Grid3 are closer to each other than in the case of Grid1 and Grid2.

From the presented numerical tests it comes out that the most accurate results were obtained using Grid3 so that it was employed in our calculations in the next Section.

4.2 Results of calculation for the finest Grid3

Figure 6 shows contours of axial and radial velocities, pressure and temperature in the nozzle and outlet regions for 500 A and 27.5 slm of argon for the finest Grid3. It was confirmed in simulations that results for the studied range of parameters are slightly fluctuating with time. The contours displayed here are static, calculated as arithmetic means of the values in 10-15 consecutive time layers with the time step of about 2-4 ms. There is some visible difference between laminar and turbulent...
flow regimes for the radial velocity and pressure, while a negligible difference for the axial velocity and temperature. The ratio of axial velocity to radial velocity is 10-30 so the bigger difference in the radial velocity practically does not influence the flow field. The displayed case is the transonic flow with the Mach number ~ 1 at the arc axis.

Figure 6. Contours of axial and radial velocities, pressure and temperature in Domain2 (extended here for the radial coordinate up to 8 mm) for 500 A and 27.5 slm of argon for the finest Grid3.

The most comprehensive result about turbulent effects for the all range of studied currents and mass flow rates is shown in figure 7, displaying the contours of the space-average relative differences (equation (9)) between laminar and turbulent flow regimes of several physical quantities calculated in Domains1, 2. To understand these plots, one must realize that calculations for laminar and turbulent flow regimes have been carried out for 16 different combinations of currents and argon mass flow rates. Each calculation provided one value of the space-average relative difference, i.e. one point in the plot. The final contours shown in figure 7 were obtained as the result of interpolation through the matrix of the discrete set of points. It can be seen that the maximum difference in Domain1 is below 2% and occurs for the Reynolds number, derived from the nozzle diameter. Domain2 exhibits higher difference up to 6% for axial velocity and therefore also for the Reynolds number. The reason for increased difference consists in steep radial gradients of temperature and velocity in the shear layer where the eddy viscosity starts to be significant. The results shown here clearly demonstrate that the plasma flow inside the discharge chamber and in the near-outlet can be regarded as quasi-laminar with negligible turbulent effects.
Finally, we compare measured and calculated radial temperature profiles 2 mm downstream of the nozzle exit for 500 A and 600 A for 22.5 slm of argon (figure 8). In our experiment, the radial profiles of the temperature near the nozzle exit were calculated from optical emission spectroscopy measurements. The procedure is based on the ratio of emission coefficients of the hydrogen Hβ line and four argon ionic lines using calculated LTE composition of the plasma for various argon mole fractions as a function of temperature [9]. It is obvious that the calculated profiles for Grids1-3 nearly overlap. Very good agreement is demonstrated between experiment and calculation for 500 A, and excellent agreement for 600 A where the measured profile nearly coincides with our calculation.

5. Conclusions
The results obtained for currents 300-600 A and for argon mass flow rates 22.5-40 slm show that:
(a) The plasma flow in the hybrid-stabilized argon-water electric arc can be regarded as quasi-laminar: The maximum space-averaged relative difference between laminar and turbulent models for each of the monitored physical quantities, calculated for the finest grid, is less than 2% within the volume of the discharge, and less that 6% for the outlet region.
(b) The proper resolution of the LES model has been reached for the finest grid (Grid3).
(c) Turbulent effects are stronger in the regions with high radial temperature and velocity gradients - near sharp edges of the outlet nozzle and in the shear layer.
(d) Comparison with available experimental temperature profiles demonstrates very good agreement for temperature radial profiles near the outlet nozzle.
Figure 8. Comparison between measured and calculated radial temperature profiles 2 mm downstream of the nozzle exit for 500 A and 600 A for 22.5 slm of argon. Turbulent flow assumption is adopted.

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