On the effect of inhomogeneous mixing of plasma species in argon–steam arc discharge

J. Jeništa[1], H. Takana[2], S. Uehara[2], H. Nishiyama[2], M. Bartlová[3], V. Aubrecht[3], A. B. Murphy[4]

[1]*Institute of Plasma Physics AS CR, v.v.i., Praha 8, Czech Republic*
[2] *Institute of Fluid Science, Tohoku University, Sendai, Miyagi, Japan*
[3]*Brno University of Technology, Brno, Czech Republic*
[4]*CSIRO Materials Science and Engineering, Lindfield, NSW, Australia*

This research focuses on numerical simulation of mixing of plasma chemical species in the discharge and near-outlet regions of the worldwide unique type of thermal plasma generator with hybrid stabilization of an electric arc by axial argon flow and tangential water vortex. The results show the effect of mixing of plasma species on the arc performance for currents 150-400 A. Calculated radial temperature and velocity profiles exhibit very good qualitative and quantitative agreements with measurements.

Keywords: arc, combined diffusion coefficients, (in)homogeneous mixing, mass fraction

1. Introduction

The so-called hybrid stabilized electric arc, developed at IPP AS CR, v.v.i. in Prague, utilizes a combination of gas and vortex stabilization. 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, which is stabilized by water vortex. The arc is attached to the external water-cooled rotating disk anode at a few millimeters downstream of the torch orifice. At present, this arc has been used for plasma spraying, pyrolysis and gasification of waste and production of syngas from biomass [1].

In our experimental configuration water species are created by evaporation of steam from a water column in the tangential direction, while argon flows axially into the discharge chamber (Fig. 1). Both gases mix inside the chamber and create plasma containing argon, oxygen and hydrogen species. It was proved from spectroscopic experiments made in IPP AS CR, v.v.i., [2] that argon and water plasma components are mixed only partially within the discharge chamber and, in addition, that mixing of individual components depends also on arc current. Since the studied plasma in the hybrid stabilized electric arc is quasi-laminar with steep radial temperature and velocity gradients [3] it can be expected that mixing and demixing processes will be important.

In the present study we investigate the effect of mixing of argon, oxygen and hydrogen plasma species on the thermal and fluid-dynamic properties of the hybrid-stabilized argon-water electric arc. The so called "combined diffusion coefficients method" [4, 5] was applied as a species mixing model. In contrast to some other authors who successfully applied this method to describe mixing of species in different arc discharges [6, 7] we consider diffusion processes due to all possible physical mechanisms (gradients of mass density, temperature, pressure, and an electric field). The results are compared with our previous calculations for the simplified assumption of homogeneous mixing [8] and with available experiments.

2. Assumptions and physical model

The following assumptions for the model are applied: 1) argon-water plasma itself is in local thermodynamic equilibrium, 2) the model is axisymmetrical (2-dimensional), 3) plasma flow is turbulent and compressible, 4) gravity effects are negligible, 5) the magnetic field is generated only by the arc itself, 6) the partial characteristics method for radiation losses is employed, 7) transport and thermodynamic properties for argon-water plasma mixture are calculated rigorously from the kinetic theory [9, 10] and they depend on temperature, pressure and argon mass fraction, 8) the combined diffusion coefficients are also functions of temperature, pressure and argon mass fraction.

Radiation losses from the argon-water arc are calculated by the partial characteristics method [11]. Continuous radiation, 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 [12]. Broadening mechanisms of atomic and ionic spectral lines due to Doppler, resonance and Stark effects have been considered. The partial characteristics are function of temperature, pressure and argon mass fraction.

Turbulence is modelled by Large eddy simulation (LES) with the Smagorinsky subgrid-scale model with the constant values of the Smagorinsky coefficient (C_S = 0.1) and the turbulent Prandtl number (Pr_t = 0.9). The Van Driest damping function near the walls is employed to suppress turbulence [13].

The resulting set of conservative governing equations for density, velocity, energy and argon mass fraction (continuity, momentum, energy and species equations) was solved numerically by the LU-SGS method [14] coupled with Newtonian iterative method. The same method was successfully applied for calculation under the assumption of homogeneous plasma mixing. To resolve compressible phenomena accurately, the Roe flux differential method [15] coupled with the third-order MUSCL-type TVD scheme [16] is used for convective term. The electric potential is calculated using the Tridiagonal Matrix Algorithm (TDMA) enforced with the block correction method.

The computer program is written in the Fortran language. The task has been solved on an oblique structured grid with nonequidistant spacing. The total number of grid points equals 193 914, with 1134 and 171 points in the axial and radial directions respectively. Calculation domain is shown in Fig. 1.

3. Details of the species mixing model

Only one species equation is required in the combined diffusion coefficients method, say for the species of gas A (argon), with the equation for argon species flux [17]:

$$\frac{\partial}{\partial t}(\rho f_A)+\nabla\cdot(\rho\vec{u}f_A)=-\nabla\cdot\vec{J}_A \quad , \qquad (1)$$

$$\vec{J}_A=-\Gamma_f\nabla f_A+\Gamma_f\frac{f_A}{M_A}\nabla M_A-\Gamma_f\frac{f_A}{M}\nabla M+$$

$$\Gamma_P\nabla(\ln P)-\bar{D}_{AB}^T\nabla(\ln T)-\Gamma_E\nabla\Phi-\frac{\mu_t}{Sc_t}\nabla f_A \ , \qquad (2)$$

where ρ is the mass density, f_A is the mass fraction of species A (gas A = argon), $\vec{J}_A$ is the argon diffusion mass flux, $\Gamma_f, \Gamma_P, \Gamma_E$ are the transport coefficients for the ordinary, pressure and electric field diffusions respectively, M_A is the average molecular weight of argon, M is the average molecular weight of all particles of gas mixture, $\bar{D}_{AB}^T$ is the combined temperature diffusion coefficient, μ_t is the eddy viscosity, Sc_t is the turbulent Schmidt number (Sc_t=1). The last term accounts for the diffusion of the argon species due to turbulence. The water species mass fraction f_B can be easily calculated from the closure condition $f_A+f_B=1$.

4. Results

Mixing of plasma species has been studied for 150–400 A and for 15.0 and 22.5 slm (standard liter per minute) of argon. The results of the model are compared with our previous *homogeneous mixing model* [8] which neglects the mixing process and assumes that argon mass fraction is constant within the whole calculation domain and determined easily from the ratio of argon to steam mass flow rates.

Some of the results are illustrated in Figs. 2-5. Comparison with the homogeneous mixing model shows the following facts: from the temperature and enthalpy contours (Figs. 2, 3) we can conclude that 1) the arc is slightly squeezed with higher temperatures at the arc axis, 2) arc fringes (low-temperature regions) are thicker, 3) enthalpy has a qualitatively different distribution within the discharge with a maximum in the nozzle region. Calculated and experimental radial temperature profiles near the nozzle exit (Fig. 4) demonstrate very good agreement if we realize that measurements have certain error bars, even though unknown in this case. Temperature was measured by optical emission spectroscopy. As for the velocity profiles (Fig. 5), measurements are very close to the calculated profiles for the present inhomogeneous mixing model. A large difference is obvious between the calculated velocity profiles for 400 A. A small asymmetry of the velocity profile (double peak) calculated by the present model for 400 A remains unexplained so far.

The other principal results not shown here can be summarized as follows:

- Mixing of water and argon plasma species is inhomogeneous under all the studied conditions (150-400A, 15-22.5 slm of argon). Argon species are dominant in the central regions of the arc, water ones in arc fringes.
- All the diffusion coefficients exhibit highly nonlinear asymmetric profiles within the discharge, depending on temperature, pressure and argon mass fraction in the plasma. The local maxima are related mostly to ionization of atoms or dissociation of steam.
- Temperature and ordinary (concentration) diffusions are the most dominant contributions in the equation for the argon mass diffusion flux. Diffusions due to pressure gradients and due to the electric field are by about one order lower.
- Compared to the homogeneous mixing model, we obtained higher reabsorption of radiation, i.e., higher arc efficiency, and lower radiation flux and its divergence (radiation losses) in the discharge.
- Qualitative agreement was also obtained for the radial argon mole fraction profiles.

5. Conclusions

The results exhibit a principal difference in enthalpy and a small difference in temperature distribution within the discharge region compared to our previous model, omitting the mixing of species. Temperature profiles for 300 and 400 A calculated by the present (inhomogeneous) and previous (homogeneous) models agree well with the experimental profiles. Agreement for the velocity profiles is much better for the inhomogeneous model.

6. Acknowledgements

The authors are grateful for the financial support under the Collaborative Research Project (J16R003) of the Institute of Fluid Science, Tohoku University, Sendai, Japan, and for their computer facilities. Our appreciation goes also to the projects GA15-19444S, GC17-10246J and GA15-14829S. Our appreciation goes also to the computational resources, provided by the CESNET LM2015042 and the CERIT Scientific Cloud LM2015085, provided under the programme ''Projects of Large Research, Development, and Innovations Infrastructures''.

7. References

[1] G Van Oost, M. Hrabovsky, V. Kopecky, M. Konrad, M. Hlina, T. Kavka, O. Chumak, E. Beckman and E.J. Verstraeten, Vacuum, **80**, 1132 (2006).
[2] M. Hrabovský, V. Kopecký, V. Sember, T. Kavka, O. Chumak and M. Konrád, IEEE Trans. Plasma Sci., **34**, 1566 (2006).
[3] J. Jeništa, H. Takana, H. Nishiyama, M. Bartlová, V. Aubrecht and P. Křenek, IEEE Trans. Plasma Sci., **42**, 2632 (2014).
[4] A.B. Murphy, Physical Review E, **48**, 3594 (1993).
[5] A.B. Murphy, J. Phys. D: Appl. Phys., **34**, R151 (2001).
[6] X. Chen and K. Cheng, Int. J. Heat and Mass Transfer, **47**, 5139 (2004).
[7] A.B. Murphy, Pure Appl. Chem., **68**, 1137 (1996).
[8] J. Jeništa, H. Takana, H. Nishiyama, M. Bartlová, V. Aubrecht, P. Křenek, M. Hrabovský, T. Kavka, V. Sember and A. Mašláni, J. Phys. D: Appl. Phys., **44**, 435204 (2011).
[9] A.B. Murphy and C.J. Arundell, Plasma Chem. Plasma Process., **14**, 451 (1994).
[10] A.B. Murphy, Plasma Chem. Plasma Process., **20**, 279 (2000).
[11] V. Aubrecht and J.J. Lowke, J. Phys. D: Appl. Phys., **27**, 2066 (1994).
[12] M. Bartlova and V. Aubrecht, Czech. J. Phys., **56**, B632 (2006).
[13] S.B. Pope, Turbulent Flows, Cambridge University Press, Cambridge 2000.
[14] A. Jameson and S. Yoon, AIAA Journal, **25**, 929 (1987).
[15] P.L. Roe, J. Comput. Phys., **43**, 357 (1981).
[16] B. Van Leer, J. Comp. Phys., **32**, 101 (1979).
[17] A.B. Murphy, Nature.com, **4**, 4304 (2014).

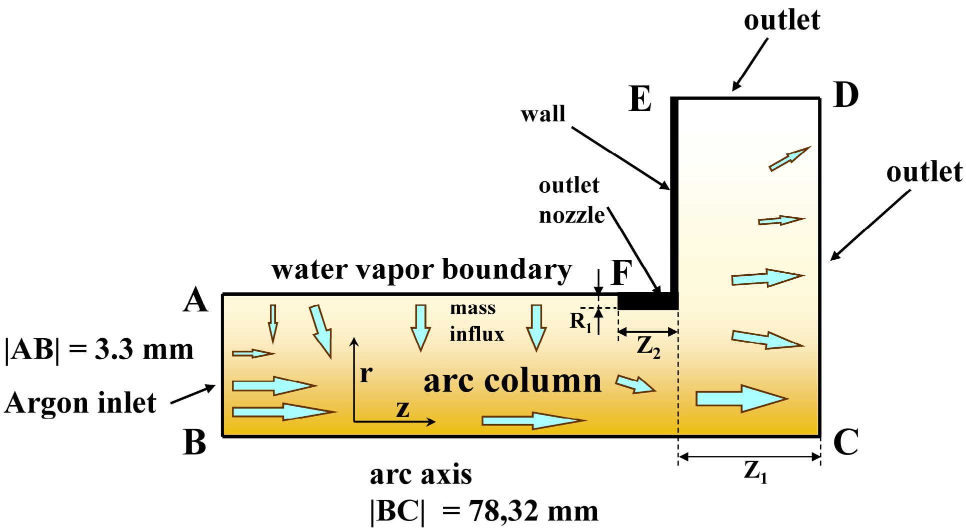

Fig. 1. Calculation domain for our problem. Argon flows axially through the AB line (+z direction) while water evaporates along the water vapor boundary AF (-r direction).

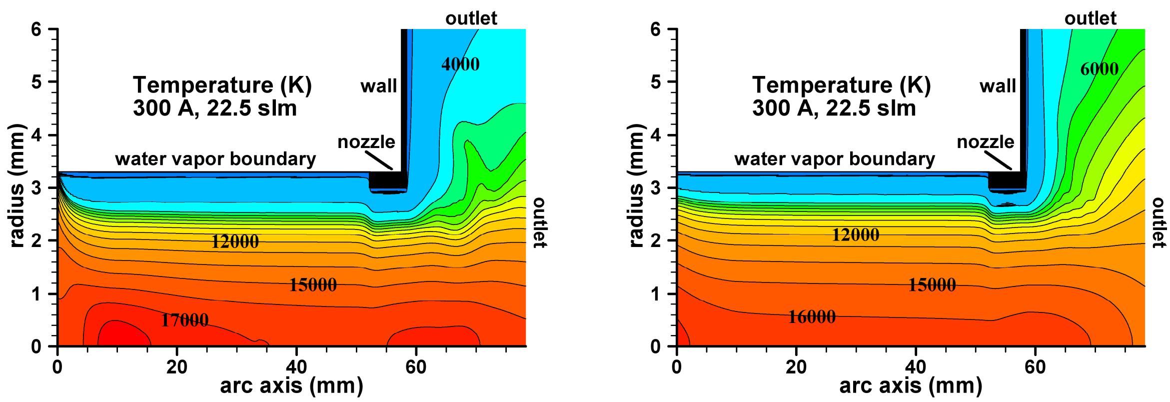

Fig. 2. Isotherms for 300 A (steam mass flow rate = 0.228 g s^{-1}) and 22.5 slm of argon. Geometry of the plot corresponds to Fig. 1. Left (right) – inhomogeneous (homogeneous) mixing model. Contour increment is 1 000 K.

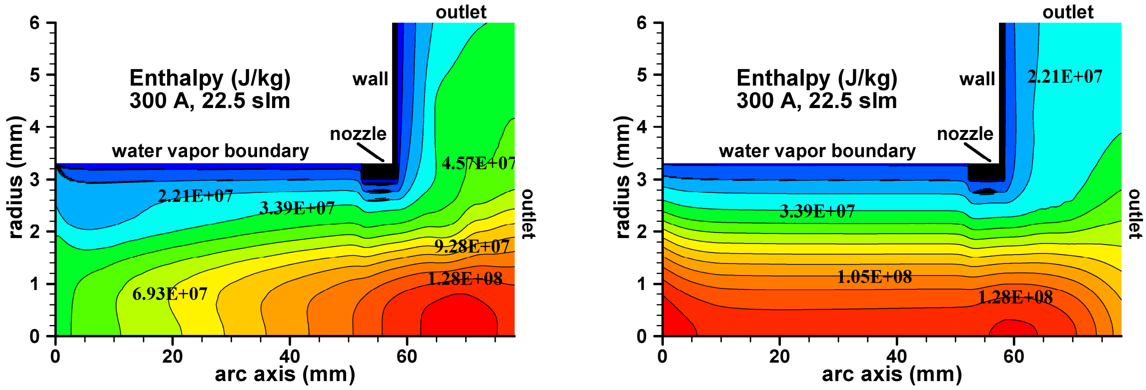

Fig. 3. Contours of enthalpy for the same conditions as in Fig. 2. Again, left (right) plot corresponds to inhomogeneous (homogeneous) mixing model.

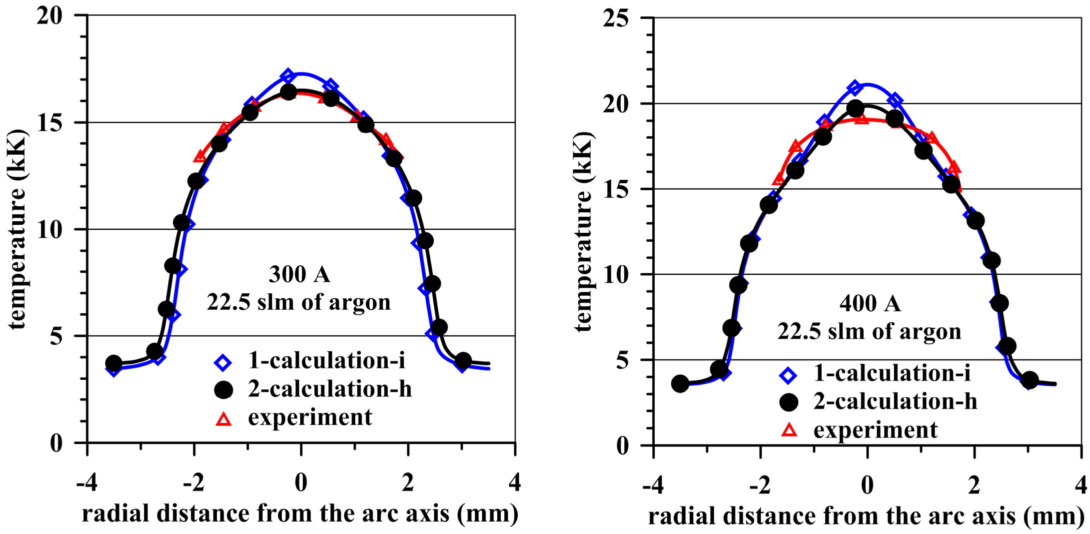

Fig. 4. Calculated and experimental radial temperature profiles 2 mm downstream of the nozzle exit. Index 'i' means inhomogeneous, index 'h' homogeneous.

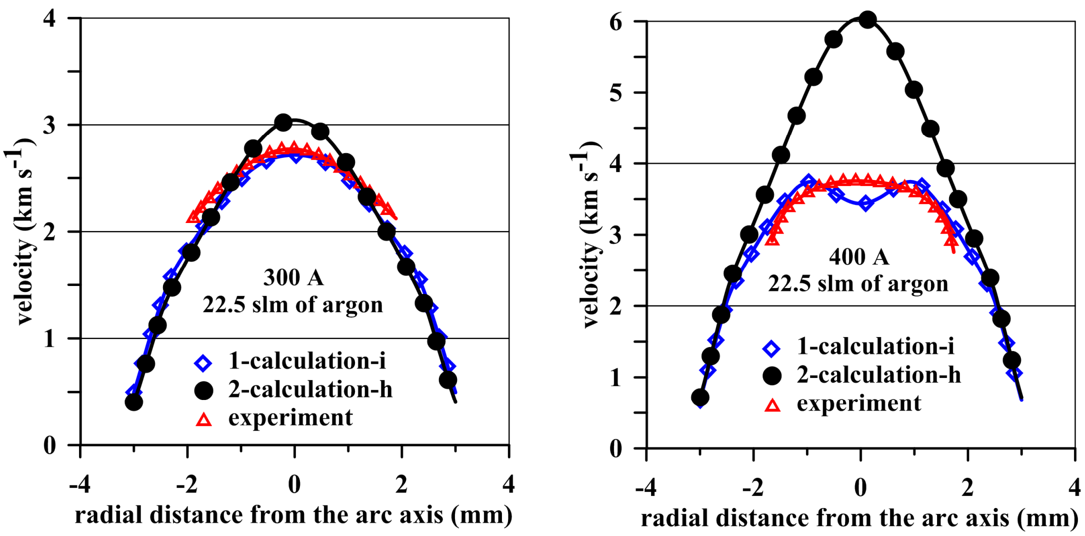

Fig. 5. Calculated and experimental radial velocity profiles 2 mm downstream of the nozzle exit with the same notation as in Fig. 4.