

The Main Issues to Address in Modeling Plasma Spray Torch Operation

Christophe Chazelas, Juan Pablo Trelles, Armelle Vardelle

▶ To cite this version:

Christophe Chazelas, Juan Pablo Trelles, Armelle Vardelle. The Main Issues to Address in Modeling Plasma Spray Torch Operation. Journal of Thermal Spray Technology, 2017, 26 (1-2), pp.3-11. 10.1007/s11666-016-0500-y. hal-01878782

HAL Id: hal-01878782 https://unilim.hal.science/hal-01878782v1

Submitted on 28 Jan 2024

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers. L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

The Main Issues to Address in Modeling Plasma Spray Torch Operation

C. Chazelas¹, J. P. Trelles², A. Vardelle¹

Abstract The modeling of plasma torch operation has advanced greatly in the last 15 years due to a better understanding of the underlying physics, development of commercial, open-source computational fluid dynamics softwares, and access to high performance and cloud computing. However, the operation mode of the electric arc in plasma torches is controlled by dynamic, thermal, electromagnetic, acoustic and chemical phenomena that take place at different scales and whose interactions are not completely understood yet. Even though no single model of plasma torch operation fully addresses these phenomena, most of these models are useful tools for parametric studies, if their use is reinforced by knowledge of torch operation and the model predictions are validated against experimental data. To increase the level of predictability of the current models, several further steps are needed. This study examines the issues remaining to be addressed in the modeling of plasma spray torch operation and the current critical aspects of these.

Keywords electric arc model · non-equilibrium model · plasma torch · torch modeling

This article is an invited paper selected from presentations at the 2016 International Thermal Spray Conference, held May 10-12, 2016, in Shanghai, P. R. China, and has been expanded from the original presentation.

A. Vardelle armelle.vardelle@unilim.fr

- University of Limoges, Limoges, France
- University of Massachusetts Lowell, Lowell, MA, USA

Introduction

Plasma spray is one of the most versatile techniques available for the application of protective and functional coatings. The processing medium is characterized by a high energy density (10⁶-10⁷ Jm⁻³) and high heat flux (10⁷-10⁹ Wm⁻²) that make it well adapted to ceramics deposition. A recent thermal spray coating market analysis by Grand View Research Inc., San Francisco predicts that ceramics coatings will be the fastest growing segment in terms of revenue at a rate of 7% for the next 7 years (Ref 1). Therefore, the use of plasma spray should expand further in particular for high temperature and extreme wear and corrosion applications.

Although plasma torches are now well-established tools in industry, they suffer from two inherent challenges during their operation: arc instability and electrode erosion. These effects limit process control and equipment lifetime, and hence adversively affect overall viability of plasma torch operation. Recent torch designs involve cascaded anode and multi-electrodes to limit the movement of the arc attachment at the anode and decrease the thermal load to electrodes. However, electrode effects still affect the process stability and economics (Ref 2). A better control of these effects requires improved understanding of the arc behavior and its effects on the plasma jet. As measurements inside plasma torches are limited to the time variation of arc voltage, inner pressure, torch thermal efficiency and acoustic emission, mathematical modeling is essential for further improvement of plasma torches.

A large body of literature deals with the modeling of plasma torch (Ref 3). Its operation is controlled by dynamic, thermal, electromagnetic, acoustic and chemical phenomena that are not fully addressed yet by the current models and several further steps are needed to achieve

calculations with a high level of predictability so that everyone, and not only those who use the models, believe them.

This paper discusses some important issues in the modeling of plasma torch operation, divided among arc-cathode interactions, arc column and arc-anode interactions. Only models that are 3D and time dependent are considered, given that they are required for the capture of the stochastic behavior of the arc. However, reduced models [e.g., steady-state (Ref 4, 5)]; dimensionality and geometry reduction; simple model of arc generation using a source term in the heat conservation equation (e.g., Ref 6) are well appropriate for plasma spray parameters optimization.

Some Remarks About Predictive Models

The plasma spray torch models have been developed and improved since the 80s (Ref 3). The first models were developed with many assumptions dealing with the torch geometry, time independency, electric current continuity between electrodes and arc, arc operation mode, thermal and chemical equilibrium, etc. If their predictions generally gave the expected trends, the more recent models that take advantage from a better knowledge in plasma torch operation and easier access to higher-performance computing resources give more accurate and detailed results: e.g., transient behavior of the arc, prediction of the electron and heavy species temperature distribution. They also make it possible to model 3-D geometry and transient mode and so, in a next future to take into account the coupling between the arc root oscillations and gas pressure variation in the cathode cavity (Ref 7). However, the challenge is now to get rid of the assumptions and imposed values that preclude to further the advances in the predictive power of plasma torch model. These main assumptions deal with simplified or incomplete torch inner geometry, imposed current density and temperature profiles at cathode tip, imposed values of cathodic and anodic voltage fall, anode attachment mode and overlasting electrodes with smooth surfaces. The use of the 3-D actual inner geometry of the plasma torch and implementation of the electrodes in the computational domain combined with electrode sheaths are believed necessary for developing NLTE (and better NCTE as discussed below) plasma torch operation models with a high predictive capability.

The ideal plasma torch model should involve the electrodes, cathode and anode regions, and arc column. The latter takes up a large part of the gas computational domain and can be considered in local thermodynamic equilibrium (LTE). Most of the current models are based on this assumption and, therefore, require some artificial treatment of the electrode-arc regions to allow the passage of the electric current. However, this assumption decreases the level of reliability and predictability of the model. A more realistic approach should take into account the departure from thermal equilibrium in the regions where the cold gas and plasma interact, as well as close to the electrodes. Such approach requires at least a two-temperature (2T) model, i.e., with the electron temperature (T_e) and heavy species temperature (T_h) , accounting for different Maxwellian speed probability distributions for electrons and heavy species, respectively. The departure from thermal equilibrium is, then, characterized by the ratio $\theta = T_e/T_h$. which can be higher than 10, as shown by the calculations of Trelles et al (Ref 8) (Fig. 1).

Near electrodes, the departure from ionization equilibrium and quasi-neutrality can be modeled by using sheath models that also make it possible to get rid of artificial boundary conditions at electrode walls. If 2T models coupling arc and electrodes using electrode sheath models have been reported for transferred arc plasma torch, e.g. (Ref 9), their application to non-transferred arc plasma

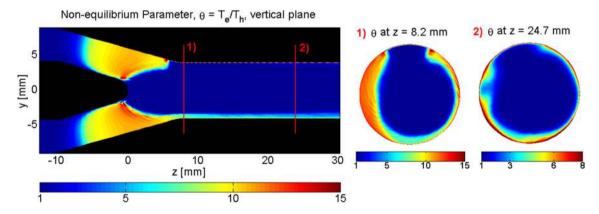


Fig. 1 Thermodynamic non-equilibrium parameter θ within an arc torch. (Conditions: gas: Ar; total current: 400 A). (Reproduced with permission from (Ref 8), copyright 2007 IOP Publishing)

spray torch is significantly more challenging due to the stochastic movement of the arc attachment at the anode wall (see "Arc-anode interactions" section). In this paper, the electrode sheath models are not presented [see for example (Ref 10, 11)], even if they are believed to be a necessary step for a fully predictive model.

Also, molecular gases (essentially N2 and H2) and gas mixtures are often used in plasma spraying to achieve plasma jets with higher enthalpy and/or velocity and ensure a better treatment of the particles injected in the plasma flow. Non-Local Chemical Equilibrium (NLCE) models should then be adopted for a better description of plasma torch operation. They require taking into account the species (including ions and electrons) of the system, possible forward and reverse chemical reactions between these species and determining the kinetic coefficients of these reactions. No plasma spray torch model so far has used NLCE models while they have already been proposed for transferred arcs (e.g., Ref 12) plasma torch operated in the transferred arc mode (Ref 13) and RF plasmas (e.g., Ref 14). They, however, generally used simplified models as stationary kinetic calculations neglecting diffusion and convection or pseudo-equilibrium approximations to limit the compute-intensive calculations.

Arc-Cathode Interactions

A large part of the current plasma spray torch numerical models consider only the gas domain with the electrodes included as boundary conditions. They impose a current density profile and a temperature on the cathode tip. The current profile has generally a Gaussian-like form:

$$J = J_0 \exp\left(-\left(\frac{r}{R}\right)\right)^n \tag{Eq 1}$$

where J is the current density over the cathode surface, r the radial coordinate measured from the torch axis and R the radius of the area on which the current density is imposed. The adjustable parameters J_0 , R and n of Eq 1 control the shape of the profile. However, under the operating conditions of plasma spray torch the arc radius and central temperature are largely dominated by the flow driven by the pinch pressure of the self-magnetic field of the arc. The latter is determined by the current density at the cathode which in turn is controlled by the geometry of the cathode and arc current. Therefore, the arc properties are largely determined by the boundary conditions that are assumed at the cathode surface as already discussed in the early 90s for stationary 2-D models of transferred arcs (Ref 15).

A way to calculate the arc behavior without imposing current density and temperature at the cathode is to include the cathode in the calculation domain; impose the arc current (j = I/S where I is the arc current and S the cathode rear cross-sectional section) and temperature at the rear face of the cathode; then calculate the heat and current density distribution in the cathode region; and include a cathode sheath model that predicts the electron and ion density and temperature at the outer boundary of the sheath as well as the cathode voltage drop.

A first step as proposed in (Ref 16) for a LTE model is to solve the electromagnetic and energy equation in the cathode region to predict the current distribution at the cathode tip and calculate the heat flux between the cathode and the arc using the following equation:

$$-k_{\rm c}\frac{\partial T_{\rm c}}{\partial z} = -k_{\rm p}\frac{\partial T_{\rm p}}{\partial z} + Q_{\rm rad} + Q_{\rm e}$$
 (Eq 2)

where z is the coordinate perpendicular to the cathode surface, the first term on the right side represents the heat transferred by conduction by the gas, the second the net radiative flux between the plasma and the cathode; and the last term the heat flux due to the thermionic cathode operation. If the cathode does not evaporate, the last term can be calculated from:

$$Q_{\rm e} = -J_{\rm em} \left(\frac{2k_{\rm B}}{e} T_{\rm c} + \Phi_{\rm c} \right) + J_i \left(\frac{2k_{\rm B}}{e} T_{\rm c} + U_{\rm c} + \Phi_i - \Phi_{\rm c} \right)$$
(Eq 3)

where the first term corresponds to the heat flux carried away by the thermionic electrons and the second the heat flux brought by the ions formed in the ionization zone that follows the cathode sheath, assuming that the heat flux brought by the back-diffusion electrons and carried away by the secondary emission electrons is negligible.

In Eq 3, Tc is the cathode surface temperature, $\Phi_{\rm c}$ the cathode material work function, $U_{\rm c}$ the cathode voltage drop, Φ_i the first ionization energy, $k_{\rm B}$ the Boltzmann constant and e the electronic charge. The electron current density $J_{\rm em}$ can be calculated from the Richardson-Dushman law (Ref 17).

Figure 2 shows the current streamlines when a current density profile is imposed on the tip of the cathode (top) and when cathode is coupled with the arc (bottom). The predicted profile of current density at the cathode tip is close to that imposed at this location when the cathode is not coupled with the arc. However, this profile results from calculations, the only input data, in that case, being the current value.

The magnetic coupling of the cathode and arc allows projecting the magnetic field both in the cathode and arc with, as expected from the Biot-Savart law, a better description of the magnetic field close to the cathode tip that directly affects the Lorentz $(\mathbf{J} \times \mathbf{B})$, where \mathbf{B} is the

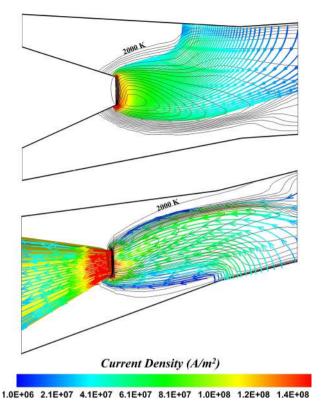


Fig. 2 Current density distribution (vector color scale) close to the cathode tip and isotherms (black lines). Operating conditions: gas: Ar-H₂; total current: 600 A; flow rate: 60 slpm; Top: with imposed current density profile at the cathode surface (predicted arc voltage: 61 V). Bottom: with arc-cathode coupling. (predicted arc voltage 72 V) (Reproduced with permission from (Ref 16), copyright 2015 Springer)

magnetic field) force and, thus, the arc velocity and finally the arc voltage.

Arc Column

The description of both the arc column and plasma jet is based on the coupling of fluid and electromagnetic equations and requires the thermodynamic (i.e., density, enthalpy and specific heat) and transport properties (viscosity, thermal and electrical conductivities and diffusion coefficients) of the gas mixture as well as its radiative properties.

Thermodynamic and Transport Properties

The calculation methods of thermodynamic and transport properties of LTE plasmas are now well established. The former require the equilibrium composition of the gas mixture, the internal partition functions and enthalpies of formation of the different species that make up the plasma gas. Some corrections (i.e., virial, Debye-Huckel) to the ideal gas law are generally taken into account.

The transport coefficients are calculated by using the Chapman-Enskog method. It should be noted that inelastic collisions are taken into account for the gas thermal conductivity ($k_{\text{tot}} = k_{\text{h}} + k_{\text{int}} + k_{\text{r}} + k_{\text{e}}$) expressed as the sum of four terms corresponding to the contribution of heavy particle translation (k_{h}), electron translation (k_{e}), internal thermal conductivity k_{int} and reaction thermal conductivity (ionization and dissociation) (k_{r}) (Ref 18).

Finally, the diffusion coefficients are now classically calculated with the method proposed by Murphy that uses combined diffusion coefficients (Ref 19). It should also be noted that the metallic vapor issued from the electrodes can significantly modify the gas properties but taking them into account requires predicting the electrode phase changes (melting, vaporization) caused by the electric arc heat load. Also the vapor can recondensate and so make the gas properties calculation difficult (Ref 20).

LTE gas properties are available for practically all gases used in plasma spraying (Ar, H₂, N₂, H₂O, He, CH₄) and their binary and ternary mixtures (Ar–H₂, Ar–He, Ar–O₂, Ar–N₂, air–N₂, air–Ar, air–O₂, air–CH₄, Ar–H₂–He, Ar–H₂–Cu) (Ref 21-26). However, the values of the interaction potentials and collision integrals that are the basis of calculations are not always well known and may lead to uncertainties in transport coefficients. Also the data must be known up to at least 30,000 K as such temperatures may appear in the calculation iterative process until the converged solution is reached.

Contrary to LTE plasmas, the 2T plasma composition and properties are still discussed in the plasma community (Ref 20). 2T plasma compositions are calculated by different models and use different relations to describe the ionization and dissociation reactions. These models include the Potapov's method, Van de Sanden et al.'s method, Gibbs free energy minimization method and kinetics model. Annaloro recently showed that the Van de Sanden's method is the best adapted to 2T plasma composition calculation (Ref 27). If there is now a generally agreed opinion on the methods of calculation of the 2T thermodynamic functions, there is still some discrepancy about the specific heat which is either calculated as a unique coefficient or divided in two coefficients for the electron and heavy particle contributions, respectively.

The 2T transport properties are calculated using essentially two approaches: the Devoto's theory (Ref 28) that does not consider the coupling between the electrons and heavy particles in the Boltzmann equation and the method by Rat that considers it (Ref 29). The Devoto's approach cannot satisfy mass conservation and the simplified expressions predict transport properties that can be quite different (especially the reactive thermal conductivity)

from those obtained with the Rat's approach. Meher (Ref 30) and Colombo (Ref 31) compared the two theories and concluded that Devoto's approach is yet adequate to determine the properties of non-equilibrium plasma. At present, the transport properties of NLTE plasmas calculated with the Devoto's model are available for some pure gases (Ar, O_2 , N_2 , H_2) and their mixtures (Ar– H_2 , Ar– O_2 , Ar– N_2 , N_2 – O_2) with electron temperature up to 45,000 K and $\theta > 15$ for some gas mixtures (Ref 31-34) while those calculated with the Rat's approach are available for Ar, Ar–He, Ar–Cu and Ar– H_2 –He plasmas but generally for $\theta < 3$. (Ref 35-37).

Recently, Wang et al. (Ref 32) showed, for a nitrogen plasma, that the ionization potential reduction due to the Coulomb interaction of charged species cannot be ignored for $\theta \geq 3$ as it affects the partition functions and, thus, the plasma composition and, thermodynamic and transport properties, as illustrated in Fig. 3 for the thermal conductivity of electrons.

Most of the current works agree on the methods of calculation of viscosity, electrical conductivity and internal and translational thermal conductivities for 2T plasmas. However, a still challenging question concerns the calculation of one or two reactional thermal conductivities, i.e., one for electrons $k_{\rm re} = k_{\rm ioni}$, and one for heavy specie $k_{\rm rh} = k_{\rm disso}$ and, consequently, the existence of a unique total thermal conductivity.

Modeling

The models limited to the gas domain solve the fluid conservation equations coupled with the Maxwell's

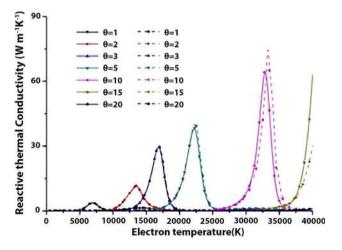


Fig. 3 Temperature dependence of the reactive thermal conductivity of nitrogen plasmas under different degrees of non-equilibrium (solid line and symbols: Debye length including only electrons; dashed line and symbols: Debye length including electrons and ions) (Reproduced with permission from (Ref 32), copyright 2011 AIP, Physics of Plasmas)

equations, while the models that include the electrodes in the computational domain solve also the energy and electromagnetic equations in electrodes. The equations are expressed in conservative form as a balance between accumulation, net flux and production as follows:

$$\frac{\partial \rho \varphi}{\partial t} + \operatorname{div}(\rho \vec{\mathbf{u}} \cdot \varphi) = \operatorname{div}(\Gamma \operatorname{grad} \varphi) + S_{\phi}$$
 (Eq 4)

with φ the conservation variable, ρ mass density, v velocity, Γ diffusion coefficient and S_{ϕ} source term.

Table 1 exemplifies the energy conservation equation. The first row shows the energy equation under LTE approximation; it corresponds to a fluid in chemical equilibrium with an internal energy characterized by a single temperature T. The second and third rows show the equivalent energy equations for a 2T model.

The LTE and NLTE equations have to be consistent; that is, the NLTE model should get reduced to the LTE model if thermal and chemical equilibrium is imposed (i.e., $T_{\rm h} = T_{\rm e.}$). Therefore, the summation of the two last rows of Table 1 must lead to the LTE equation given in the first row. In the NLTE model, the electron and heavy particle energy equations involve well-known terms, but the expressions of these terms rise some questions: What is the proportion of radiation due to electrons and heavy particles for a given temperature range? What is the role of the electrons on the reactional thermal conductivity? What is the role of the heavy particles in dissociation processes? These questions lead to different formulations of energy equations (Ref 39) that differ in the distribution of reactive thermal conductivity and ionization term in the two equations. The right formulation should result in departure from thermal equilibrium with $\theta \ge 1$, and T_e should be higher than T, the predicted LTE temperature, while $T_{\rm h}$ should be lower than T.

An example of the arc shape predicted by a 2T model together with the distribution of electric potential is given in Fig. 4 (Ref 40). The use of a NLTE model allows a better description of plasma flow, especially closed to the electrodes and in the arc column fringes, where steep gradients of temperature take place. This approach results in a better evaluation of the electrical conductivity near the electrodes, leading to a decrease in the arc electrical resistivity and thus in the predicted arc voltage.

The solution of the set of conservation equations requires appropriate boundary conditions, some of which are not straightforward to be chosen, e.g., as the temperature of the electrons $T_{\rm e}$ at the torch inlet in a 2T model or the value of the magnetic vector potential $\bf A$ when the potential vector formulation is used to compute the electromagnetic field (Ref 41). Also, if the computational domain is limited to the torch itself, special care is needed at the nozzle exit to ensure the uninterrupted progress of

Table 1 Plasma energy conservation equations in LTE and non-LTE conditions

Conservation	Accumulation	Net flux	Net production
Conservation equation of energy for a local thermal equilibrium plasma (LTE)			
Int, energy	$\frac{\partial \rho h}{\partial t}$	$\nabla \cdot (\mathbf{u}\rho h{+}\mathbf{q}')$	$\frac{Dp}{Dt} - \mathbf{\tau} : \nabla_{\mathbf{u}} + \mathbf{J}_q \cdot (\mathbf{E} + \mathbf{u} \times \mathbf{B}) - \dot{Q}_r$
Conservation equation of energy for a non-local thermal equilibrium plasma (NLTE)			
Int, energy electrons	$\frac{\partial \rho h_h}{\partial t}$	$\nabla \cdot \left(\mathbf{u} ho h_h + \mathbf{q}_h' ight)$	$rac{Dp_h}{Dt} - au : abla_{f u} + \dot{Q}_{eh}$
Int, energy heavy species	$\frac{\partial \rho h_e}{\partial t}$	$ abla \cdot \left(\mathbf{u} ho h_e {+} \mathbf{q}_e' ight)$	$\frac{Dp_e}{Dt}$ + $\mathbf{J}_q \cdot (\mathbf{E} + \mathbf{u} \times \mathbf{B}) - \dot{Q}_r - \dot{Q}_{eh}$

 $^{{\}bf q}'$ Represent total diffusive fluxes; ${\bf Q}_r$ is the net emission coefficient and ${\bf Q}_{eh}$ the energy exchange term between electrons and heavy particles (Ref 3, 8, 38) and the indices e and h denote heavy species and electrons, respectively

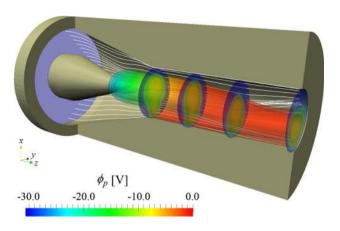


Fig. 4 Snapshot of voltage distribution over heavy species temperature slices and iso-surface 8, 12 and 16 kK approximately predicted with a 2T model for argon plasma at 400 A. The arc voltage is around 30 V compared to 50 V for LTE predictions under the same plasma conditions. (Reproduced with permission from (Ref 40), copyright 2014 Elsevier Publishing.)

the flow characteristics out of the computational domain. A recommended method is the use of absorbing layers or sponge zones to attenuate the outgoing waves and decay any reflected wave as it travels through the absorbing layer (Ref 3).

Finally, an issue that has still to be addressed is the coupling between the gas pressure variation in the plasma torch and the voltage variation. Rat et al have shown (Ref 7) that some compressibility effects of the plasma-forming gas in the cathode cavity can bring about acoustic resonance phenomena because of a reciprocal dependence of arc voltage and pressure inside the cavity that contains the cold plasma-forming gas. When the position of the anode arc attachment varies, the plasma-forming gas pressure and flow rate change, and thus the plasma flow. To predict the effect of acoustic waves on the torch operation mode, the numerical model should take into account the actual inner geometry of the torch, compressibility of the gas and couple the fluid and acoustic equations. To the best of our knowledge, this effect has not been numerically studied yet, despite the use of compressible plasma models.

Arc-Anode Interactions

The modeling of the interaction of the plasma inside the torch with the surrounding anode has to address three main aspects: (1) the displacement of the arc-anode attachment, (2) the arc reattachment process, and (3) the phenomena at the plasma-anode interface.

Displacement of the Arc-Anode Attachment

The dynamics of the arc inside the torch can be discerned through two main features: the movement of the arc-anode attachment and the process of formation of a new arc-anode attachment, that what is called the arc reattachment process (Ref 3, 42, 43). The dynamic nature of the arc is evidenced by the temporal variation of the voltage drop between the electrodes, as well as by fluctuations in the temperature, pressure and velocity at the torch exit.

Representative simulation results of the voltage drop signal $(\Delta\phi)$ together with snapshots of the temperature distribution inside a typical DC arc plasma torch are shown in Fig. 5. The simulations were based on a thermodynamic non-equilibrium (NLTE) plasma flow model. Details about the model, its numerical implementation, and validation, including its comparison against a thermodynamic equilibrium (LTE) model, are found in (Ref 8, 38).

The results in Fig. 5 depict the displacement of arcanode attachment and arc reattachment process. The displacement of the anode attachment is a direct consequence of the imbalance between the drag force due to the interaction of the working gas flow on the plasma and the electromagnetic (Lorentz) force caused by the local curvature of the arc. The dominance of the drag force causes the displacement of the arc-anode attachment along the direction of the flow, linearly in the case of straight injection. The displacement of the arc-anode attachment is depicted in Fig. 5 (top) by the variation in $\Delta \phi$ between the points a and b, as well as in the temperature distribution snapshots in Fig. 5 (bottom) by comparing the locations of

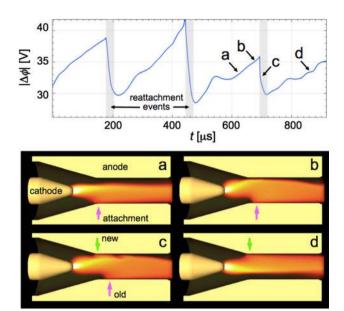


Fig. 5 Arc dynamics and arc reattachment events. (Top) Time evolution of the voltage difference $(\Delta\phi)$ across the torch depicting the occurrence of three arc reattachments events. (Bottom) temperature field snapshots at representative instants: (a)—single established anode attachment; (b)—dragging of the attachment along the flow direction; (c)—formation of a new attachment, which is more thermodynamically favorable due to its proximity to the cathode; and (d)—predominance of the new attachment and extinguishment of the old one. (Conditions: gas: Ar; total current: 400 A; flow rate: 60 slpm; diameter at torch exit: 8 mm) (Ref 38)

the anode attachment (indicated by the arrows) in frame ${\bf a}$ with respect to that in frame ${\bf b}$.

The description of the displacement of the anode attachment requires the accurate and concurrent solution of the equations of the fluid dynamic model (incompressible or compressible flow, in chemical and thermodynamic equilibrium or non-equilibrium) together with those describing the evolution of the (self-induced) electromagnetic field (Maxwell's equations) in a time-dependent and three-dimensional domain, despite the constancy and axisymmetry of operating conditions and torch geometry.

Arc Reattachment and Electrical Breakdown

A major challenge for the modeling of plasma spray torch operation is the capture of reattachment events. These events consist of the formation of a new electrical connection between the arc and the anode and are manifested externally by a relatively sudden decrease in voltage drop, as observed in Fig. 5. Although the exact mechanisms driving the reattachment process are not completely understood, the relatively high electric fields, together with the abundance of excited species around the arc (by UV excitation), and the short-time scale of the process, suggest that the arc reattachment can be initiated by a streamer-like

breakdown or some small portion of the current flowing behind the main arc attachment (Ref 44). This streamer connects the arc with the anode in a region somewhere upstream of the existing arc attachment, creating a conducting channel that allows the establishment of a new arc attachment. The detailed modeling of a streamer-like reattachment event involves a wide range of spatial and temporal scales (i.e., high spatial and temporal resolution in order to capture the streamer initiation and propagation) and requires an increase in the complexity of the physical model (i.e., chemical non-equilibrium due to the rapid temporal variations, photon-driven ionization, and potentially without the assumption of charge neutrality). Although the high spatial resolution and detailed physical model to describe a streamer are mainly needed in the breakdown region, such region is not known beforehand; and the use of such high-resolution and detailed model throughout the plasma torch domain is practically unfeasible with actual computational methods and computer power, especially within a realistic simulation of plasma spray torch operation. Therefore, approximate models have been used to describe it; they mimic the relatively spontaneous formation of the new conducting channel, e.g. (Ref 45, 46).

Alternative to breakdown-like events, a new anode attachment can form whenever a section of the arc column gets in close proximity to the anode surface. In such situation, the high temperatures, and hence high electrical conductivity, characteristic of the regions near the arc promote the establishment of new electrically conducting path. Such events have also been captured by plasma torch simulations; i.e., by the use of an artificially high electrically conductivity all along the anode surface in the case of LTE models, or by relying on the more diffusive nature of the electron temperature field in NLTE models (Ref 8).

Plasma-Anode Interface

An accurate description of the plasma-anode interface is very involved and encompasses complex thermal, electromagnetic, and material transport phenomena (i.e., heat transfer, current transfer and potential material transport in the case of anode erosion (Ref 40), respectively).

For example, the heat transfer to the anode Q_a can be given by:

$$\begin{split} Q_{a} &= -k_{h}\frac{\partial T_{h}}{\partial z} - k_{e}\frac{\partial T_{e}}{\partial z} + Q_{e} + J_{qe}W_{a} + J_{qi}(E_{i} \\ &- W_{a}) + Q_{rad} \end{split} \tag{Eq 5}$$

where z is in the direction normal to the anode, $k_{\rm h}$ and $k_{\rm e}$ are the heavy species (atoms, ions) and electron thermal conductivity, respectively; $T_{\rm h}$ and $T_{\rm e}$ the heavy species and electron temperatures; $J_{\rm qe}$ and $J_{\rm qi}$ are the electron and ion

current densities, $Q_{\rm e}$ is the transport of energy by the electron flux often defined as $Q_{\rm e} = J_{\rm qe}(h_{\rm e}/e - {\rm U_a})$, where ${\rm h_e}$ is the electron enthalpy, e the elementary charge, and $U_{\rm a}$ the voltage drop across the anode sheath; $W_{\rm a}$ is the work function of the anode material, $E_{\rm i}$ is the ionization energy of the ion, and $Q_{\rm rad}$ is the radiative heat flux to the anode (Ref 3).

Typically, the first, third and fourth terms are the most important ones, and hence $Q_{\rm a}$ depends significantly on $J_{\rm qe}$. For NLTE models, the boundary conditions for $T_{\rm h}$ and $T_{\rm e}$ should be obtained by splitting Eq 5, i.e., the terms involving electrons specify the boundary condition for $T_{\rm e}$, and the others the condition for $T_{\rm h}$. The expression for $Q_{\rm a}$ in Eq 5 has to be extended to include anode material modifications, such as erosion or surface reactions, which could significantly affect the overall heat transferred.

Additionally, the accurate description of the arc-anode interface requires an adequate account of the heat transfer and current transfer through the anode domain, e.g., to describe the removal of heat from the plasma by the cooling water and the transport of current from the arc to the electric terminals connecting the anode. Such description requires incorporating, at least partially, part of the anode within the computational domain of the simulation, which can significantly increase model complexity and the computational cost of simulation (as described in "Arc-Cathode Interactions" section).

Conclusion

If the current LTE spray torch models are useful for parametric studies, they have to be developed further (in a sequential approach) to yield reliable and predictive calculations. 2T models have proved to be necessary to better describe the arc column fringes and electrode regions and predict more realistically the arc voltage. However, some questions remain about the 2T transport properties and in particular the thermal reactive conductivity and radiation of electrons and heavy particles over specific temperature ranges. The main improvements needed include the coupling of electrodes and arc with the solution of electromagnetic and energy equations in both electrodes and the incorporation of electrode sheath models. The current developments in specific fields like plasma welding, cutting and HID lamps can help to develop such models. However, a specific issue in plasma spray torch modeling that is not addressed in transferred arc models is the movement of the arc attachment at the anode wall that makes the implementation of an anode sheath model much more complex. As a first step, the model could be developed for a plasma torch with a single cathode and a cascaded anode geometry that consists of a stack of copper rings insulated from each other and ending with an anode ring on which the arc attaches. This geometry restricts the movement of the arc to the anode ring, and the arc could be modeled as a transferred arc with an imposed attachment point in order to get rid of the problem of the implementation of the anode in the computational domain and anode sheath with a model of arc reattachment events.

At the end, such models could predict the phase change in electrodes and time erosion. Finally, the coupling of the arc dynamics with the propagation of the acoustic waves generated by the compressibility effect of the plasmaforming gas in the cathode cavity should allow for better control of the arc instabilities. This coupling could be investigated first with the current compressible plasma models limited to the gas domain.

References

- 1. Thermal Spray Coating Market Analysis, Grand View Research Inc., San Francisco (2015), ISBN Code: 978-1-68038-514-4
- A. Vardelle, C. Moreau, N.J. Themelis, and C. Chazelas, A Perspective on Plasma Spray Technology, *Plasma Chem. Plasma Process.*, 2015, 35(3), p 491-509
- J. P. Trelles, C. Chazelas, A. Vardelle, and J. V. R. Heberlein, Arc Plasma Torch Modeling. J. Therm. Spray Technol., 2009, 18(5/6), p 728-752
- K. Bobzin and M. Öte, Modeling Multi-Arc Spraying Systems, J. Therm. Spray Technol., 2016, 25(5), p 920-932
- K. Bobzin, M. Öte, J. Schein et al., Modelling the Plasma Jet in Multi-Arc Plasma Spraying, J. Therm. Spray Technol., 2016, 25(6), p 1111-1126
- G. Mariaux and A. Vardelle, 3-D Time-Dependent Modelling of the Plasma Spray Process: Part 1—Flow Modelling, *Int. J. Therm. Sci.*, 2005, 44, p 357-366
- V. Rat and J.F. Coudert, Acoustic Stabilization of Electric Arc Instabilities in Non-transferred Plasma Torches, *Appl. Phys. Lett.*, 2010, 96, p 101503
- 8. J.P. Trelles, E. Pfender, and J.V.R. Heberlein, Non-equilibrium Modeling of Arc Plasma Torches, *J. Phys. D Appl. Phys.*, 2007, **40**(19), p 5937-5952
- J. Wendelstorf, Ab Initio Modelling of Thermal Plasma Gas Discharges. Ph.D. Thesis, 2000, Carolo-Wilhelmina University, Germany
- M.S. Benilov, Understanding and Modelling Plasma-Electrode Interaction in High-Pressure Arc Discharges: A Review, *J. Phys.* D Appl. Phys., 2008, 41(14), p 144001
- M.S. Benilov, N.A. Almeida, M. Baeva, M.D. Cunha, L.G. Benilova, and D. Uhrlandt, Account of Near-Cathode Sheath in Numerical Models of High-Pressure Arc Discharges, *J. Phys. D Appl. Phys.*, 2016, 49(21), p 215201
- M. Baeva, R. Kozakov, S. Gorchakov, and D. Uhrlandt, Two-Temperature Chemically Non-equilibrium Modeling of Transferred Arcs, *Plasma Sources Sci. Technol.*, 2012, 21, p 055027
- S. Ghorui and A.K. Das, Exploring Chemical and Thermal Nonequilibrium in Nitrogen Arcs, J. Phys: Conf. Ser., 2012, 406, p 012012
- R. Ye, A.B. Murphy, and T. Ishigaki, Numerical Modeling of an Ar-H₂ RF Plasma Reactor Under Thermal and Chemical Nonequilibrium Conditions, *Plasma Chem. Plasma Process.*, 2007, 27, p 189-204

- P. Zhu, J.J. Lowke, and R. Morrow, A Unified Theory of Free Burning Arcs, Cathode Sheaths and Cathodes, *J. Phys. D Appl. Phys.*, 1992, 25(8), p 1221-1230
- M. Alaya, C. Chazelas, G. Mariaux, and A. Vardelle, Arc-Cathode Coupling in the Modeling of a Conventional DC Plasma Spray Torch, J. Therm. Spray Technol., 2015, 24(1-2), p 3-10
- S. Coulombe and J.L. Meunier, A Comparison of the Electron-Emission EQUATION used in Arc-Cathode Interaction Calculations, J. Phys. D Appl. Phys., 1997, 30, p 2905-2910
- Y. Cressault, Basic Knowledge on Radiative and Transport Properties to Begin in Thermal Plasmas Modelling, AIP Adv., 2015, 5, p 057112
- A.B. Murphy, Diffusion in Equilibrium Mixture of ionized Gases, *Phys. Rev. E*, 1993, 48(5), p 3594
- 20. A. Gleizes, Perspectives on Thermal Plasma Modelling, *Plasma Chem. Plasma Process.*, 2015, **35**(3), p 455-469
- A.B. Murphy, Transport Coefficients of Hydrogen and Argon-Hydrogen Plasmas, *Plasma Chem. Plasma Process.*, 2000, 20(3), p 279-297
- A.B. Murphy, Transport Coefficients of Air, Argon-Air, Nitrogen-Air, and Oxygen-Air Plasmas, *Plasma Chem. Plasma Process.*, 1995, 15(2), p 279-307
- A.B. Murphy and C.J. Arundelli, Transport Coefficients of Argon, Nitrogen, Oxygen, Argon-Nitrogen, and Argon-Oxygen Plasmas, *Plasma Chem. Plasma Process.*, 1994, 14(4), p 451-490
- B. Sourd, J. Aubreton, M.F. Elchinger, M. Labrot, and U. Michon, High Temperature Transport Coefficients in e/C/H/N/O Mixtures, J. Phys. D Appl. Phys., 2006, 39(6), p 1105-1119
- A.B. Murphy, Transport Coefficients of Hydrogen and Argon-Hydrogen Plasmas, *Plasma Chem. Plasma Process.*, 2000, 20(3), p 279-297
- Y. Cressault and A. Gleizes, Thermodynamic Properties and Transport Coefficients in Ar-H₂-Cu Plasma, J. Phys. D Appl. Phys., 2004, 37(4), p 560-572
- 27. J. Annaloro, P. Teulet, A. Bultel, Y. Cressault, and A. Gleizes, Calculation of Composition and Thermodynamic Properties in Thermal Non-equilibrium Conditions, in 13th *International* Conference High Technology Plasma, 22-27 June 2014, Toulouse, France
- M.I. Boulos, P. Fauchais, and E. Pfender, Thermal Plasmas: Fundamentals and Applications, Plenum Press, New York, 1994
- V. Rat, P. André, J. Aubreton, M.F. Elchinger, P. Fauchais, and A. Lefort, Transport Properties in a Two-Temperature Plasma: Theory and Application, *Phys. Rev. E*, 2001, 64(2), p 026409
- K.C. Meher, N. Tiwari, and S. Ghorui, Thermodynamic and Transport Properties of Nitrogen Plasma Under Thermal Equilibrium and Non-equilibrium Conditions, *Plasma Chem. Plasma Process.*, 2015, 35(4), p 605-637
- V. Colombo, E. Ghedini, and P. Sanibondi, Thermodynamic and Transport Properties in Non-equilibrium Argon, Oxygen and

- Nitrogen Thermal Plasmas, *Prog. Nucl. Energy*, 2008, **50**, p 921-933
- W.Z. Wang, M.Z. Rong, J.D. Yan, A.B. Murphy, and J.W. Spencer, Thermophysical Properties of Nitrogen Plasmas Under Thermal Equilibrium and Non-equilibrium Conditions, *Phys. Plasma*, 2011, 18, p 113502
- S. Ghorui, J. Heberlein, and E. Pfender, Thermodynamic and Transport Properties of Two-Temperature Oxygen Plasmas, Plasma Chem. Plasma Process., 2007, 27(3), p 267-291
- V. Colombo, E. Ghedini, and P. Sanibondi, Two-Temperature Thermodynamic and Transport Properties of Argon-Hydrogen and Nitrogen-Hydrogen Plasmas, J. Phys. D Appl. Phys., 2009, 42(5), p 055213
- 35. J. Aubreton, M.F. Elechinger, P. Fauchais, V. Rat, and P. André, Thermodynamic and Transport Properties of a Ternary Ar-H₂-He Mixture Out of Equilibrium up to 30 000 K at Atmospheric Pressure, J. Phys. D Appl. Phys., 2004, 37(16), p 2232-2246
- J. Aubreton, M.F. Elchinger, V. Rat, and P. Fauchais, Two-Temperature Transport Coefficients in Argon-Helium Thermal Plasmas, J. Phys. D Appl. Phys., 2004, 37(1), p 34-41
- J. Aubreton and M.F. Elchinger, Transport Properties in Non-equilibrium Argon, Copper and Argon-Copper Thermal Plasmas,
 J. Phys. D Appl. Phys., 2003, 36(15), p 1798-1805
- J.P. Trelles, Computational Study of Flow Dynamics from a DC Arc Plasma Jet, J. Phys. D Appl. Phys., 2013, 46(25), p 255201
- P. Freton, J.J. Gonzalez, Z. Ranarijaona, and J. Mougenot, Energy Equation Formulations for Two-Temperature Modelling of 'Thermal' Plasmas, J. Phys. D Appl. Phys., 2012, 45(46), p 465206
- J.P. Trelles and S.M. Modir Khazeni, Variational Multiscale Method for Nonequilibrium Plasma Flows, *Comput. Methods Appl. Mech. Eng.*, 2014, 282, p 87-131
- P. Freton, J.J. Gonzalez, M. Masquère, and F. Reichert, Magnetic Field Approaches in DC Thermal Plasma Modelling, *J. Phys.* D Appl. Phys., 2011, 44(34), p 345202
- 42. C. Baudry, A. Vardelle, and G. Mariaux, Numerical Modeling of a DC Non-transferred Plasma Torch: Movement of the Arc Anode Attachment and Resulting Anode Erosion, *High Temp. Plasma Process.*, 2005, **9**, p 1-15
- C. Chazelas, E. Moreau, G. Mariaux, and A. Vardelle, Numerical Modeling of Arc Behavior in a DC Plasma Torch, *High Temp. Mater. Process.*, 2006, 10, p 393-406
- V.A. Nemchinsky, On Conductivity of Cold Gas Layer Separating Arc Column and Nozzle in Nontransferred Plasma Arc, *IEEE Trans. Plasma Sci.*, 2015, 43, p 2715-2721
- 45. E. Moreau, C. Chazelas, G. Mariaux, and A. Vardelle, Modeling of the Restrike Mode Operation of a DC Plasma Spray Torch, *J. Therm. Spray Technol.*, 2006, **15**(4), p 524-530
- J.P. Trelles, E. Pfender, and J.V.R. Heberlein, Modeling of the Arc Reattachment Process in Plasma Torches, J. Phys. D Appl. Phys., 2007, 40(18), p 5635-5648