Numerical Analysis of Ar and Ar-H2 Atmospheric Plasma Spray With a Simplified Model

Chao Tan, Ji Li

School of Physics and Electronic Engineering, Fuyang Normal University, Fu Yang, An Hui 236037, China

Abstract. To study the difference of plasma spraying process between argon and argon-hydrogen working gas, a relative simplified fan-shaped numerical model of argon/argon-hydrogen atmospheric plasma spray process was set up to analyze the multi-physic field in the spraying gun. The model took electrodes especially cathode and anode boundary layers into consideration. In other words, a two-temperature plasma model was employed. With regard of both ionization and recombination of ions and electrons, their number density distributions, which are important to determine whether the injected particles are charged, were studied. The influence of secondary gas on plasma flow was investigated. According to the results, when adding hydrogen into the pure argon plasma, the temperature and velocity of the gas flow in spray gun chamber increased. The calculated results will provide theoretical guidance for the design and optimization of gun structure.

1. Introduction

Atmospheric plasma spraying has been used in fabrication of high performance coatings. Since thermal plasma processing is, in general, governed by a large number of parameters, implementation of controls becomes mandatory. The lack of sufficient controls combined with economic drawbacks in some cases has been the main obstacle for the growth of thermal plasma technology [1]. For several years, continues efforts have been conducted to get the highest reproducibility of high-level properties coatings by Huang et al.[2] and Mauer et al.[3], which requires firstly to know the gas flow behavior both in and out of the spraying gun [4].

With the rapid development of computer technology, Selvan and Ramachandran adopted 3D model to analysis heat transfer and fluid flow in plasma spray process[5]. Those models frequently used for simulations of plasma spray torches relied on the local thermodynamic equilibrium (LTE) approximation by Trelles et al. [6,7]. And then Huang regarded the plasma flow as a property-varying electromagnetic reactive fluid in a state of chemical equilibrium, in which the internal energy of the fluid was characterized by the single parameter of gas temperature[8]. There are few reports of model including gun electrodes and discussion of added hydrogen influence on the argon plasma spraying.

In this paper, a fan-shaped simplified model including the whole gun geometry was introduced to study the added hydrogen influence on the plasma flow. The highly non-equilibrium region very close to the cathode and anode, including the space-charge sheath and the ionization pre-sheath, has been considered in this work. A two temperature model was used to compute the ion and electron temperature. With reaction rates defined, the chemical non-equilibrium was considered.
2. Model Methodology

2.1. Governing equations

As a continuum gas, the continuity equation reflects the continuum medium assumption. The physical meaning of this equation is that the fluid will occupy continuously every point of the space in the flow domain.

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

(1)

where \( \rho \) is gas density, \( \vec{V} \) is velocity magnitude.

The momentum equation links the flow velocity of a fluid element with the external forces acting on it.

\[
\frac{\partial (\rho \vec{V})}{\partial t} + \nabla \cdot (\rho \vec{V} \vec{V}) = -\nabla P + \nabla \cdot \vec{\tau}
\]  

(2)

where \( \rho \) is gas density, \( \vec{\tau} \) is shear stress tensor,

For the heavy species, its temperature and enthalpy is governed by energy equation:

\[
\frac{\partial (\rho H)}{\partial t} + \nabla \cdot (\rho \vec{V} H) = \nabla \cdot (k \nabla T) + \frac{DP}{Dt} - S_R
\]  

(3)

where \( k \) is thermal conductivity of plasma, \( P \) is pressure, \( S_R \) is the source term (such as Joule heating and radiation). The enthalpy \( H \) is defined as:

\[
H = h + \frac{1}{2} V^2
\]  

(4)

where \( h \) is the internal energy.

Take the ideal gas equation:

\[
P_w = \rho RT
\]  

(5)

where \( w \) is the species or mixture molecular weight, \( R \) is perfect gas constant.

For the gas flow calculation, the \( k-\varepsilon \) model is employed in this study.

\[
\frac{\partial (\rho k_i)}{\partial t} + \nabla \cdot (\rho \vec{V} k_i) = \nabla \cdot ((\mu + \frac{H_i}{\sigma_k}) \nabla k_i) + G_i - \rho \varepsilon
\]  

(6)

\[
\frac{\partial (\rho \varepsilon)}{\partial t} + \nabla \cdot (\rho \vec{V} \varepsilon) = \nabla \cdot ((\mu + \frac{H_i}{\sigma_\varepsilon}) \nabla \varepsilon) + c_\mu G_i \frac{\varepsilon}{k_i} - c_{\varepsilon 2} \rho \frac{\varepsilon^2}{k_i}
\]  

(7)

\[
\mu_t = c_\mu \rho \frac{k_i^2}{\varepsilon}
\]  

(8)

where \( k_i \) is turbulence energy, \( \varepsilon \) is turbulent dissipation rate, \( \mu_t \) is the turbulent viscosity.

For the conduction in cathode and anode solid as well as the conductive plasma flow are governed by the current continuity equation:

\[
\frac{\partial \rho_c}{\partial t} + \nabla \cdot \vec{J} = 0
\]  

(9)

where \( \rho_c \) is the charge density and \( \vec{J} \) is the electric current density.

In DC conduction we solve the Laplace equation:

\[
\nabla \cdot (\sigma \nabla \phi) = 0
\]  

(10)

where \( \sigma \) is electrical conductivity, \( \phi \) is electric potential.

The electric field \( \vec{E} \) is computed as:
\[ \mathbf{E} = \nabla \phi \]  
\[ (11) \]

For magnetic \( \mathbf{B} \) field, the governed equations are Maxwell-Faraday equations:
\[ \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \]
\[ (12) \]

In the heating zone, Ohm’s law is applied:
\[ P_{\text{Joule}} = J \mathbf{E} \]
\[ (13) \]

2.2. Computational model and plasma reactions

When the outer powder injector is eliminated, the atmospheric gun displays a three dimensional symmetry geometry about the axis. So a fan-shaped model, which represents the whole gun structure, was employed in this study. The computational model is displayed in Figure 1.

![Computational model of plasma spray](image)

**Figure 1.** Computational model of plasma spray

There were 56800 computational nodes and 42892 cells in this kind of model. As described in the figure, the anode and cathode were included. And electrodes boundary layers between the arc column and the metallic electrodes were took into consideration. Besides, considering different computational resources needed between outer space and gun chamber, the mesh densities of these two domains were different; the inner mesh was denser than that of outer. On the interface between solid and fluid, the mesh density was enhanced too.

In this paper, the kinetic model was applied to obtain plasma compositions. This model, provided all reactions and coefficients are known, gives realistic species compositions. However the reactions of the ionization and recombination are complex, so only some dominating reactions and species were considered in a numerical model. When there was only argon work in the gun, the following reactions and species were taken into account:

- Activation of argon: \( \text{Ar} + e \rightarrow \text{Ar}^* + e \)
- Ionization of argon: \( \text{Ar} + e \rightarrow \text{Ar}^* + 2e \)
- Recombination of argon: \( \text{Ar}^* + 2e \rightarrow \text{Ar} + e \)

When hydrogen was added with a volume fraction of 20%, additional reactions shown below were considered:

- Dissociation of H2: \( 2\text{H} + \text{H}_2 \rightarrow 2\text{H}_2, \ 3\text{H} \rightarrow \text{H}_2 + \text{H} \), \( e + \text{H}_2 \rightarrow 2\text{H} + e \), \( 2\text{H} + \text{Ar} \rightarrow \text{H}_2 + \text{Ar} \);
- Ionizations: \( e + \text{H} \rightarrow \text{H}^* + 2e \), \( e + \text{H}_2 \rightarrow \text{H}_2^* + 2e \);
- Recombination: \( e + \text{H}_2^* \rightarrow 2\text{H}, \ e + \text{ArH}^* \rightarrow \text{ArH} + \text{H} \)
- Charge transfer: \( \text{H}^* + \text{H}_2 \rightarrow \text{H} + \text{H}_2^*, \ \text{Ar}^* + \text{H}_2 \rightarrow \text{Ar} + \text{H}_2^*, \ \text{Ar}^* + \text{H}_2 \rightarrow \text{ArH}^* + \text{H} \)

2.3. Computational settings

The computational conditions listed in Table 1 were all extracted from the realistic application of spraying parameters.
Table 1. Computational conditions of Atmospheric Plasma Spraying

| Parameters                              | Value          |
|-----------------------------------------|----------------|
| Gun diameter                            | 7 [mm]         |
| Length of the gun                       | 32.5 [mm]      |
| Density computation method              | Ideal Gas Law  |
| Diameter of the ambient domain          | 35.5 [mm]      |
| Length of the ambient domain            | 160 [mm]       |
| Outer space pressure                    | 1 [atm] (0.1 [MPa]) |
| Model of turbulence                     | RNG k-ε        |
| Viscosity method                        | Sutherland Law |
| Specific Heat method                    | JANNAF Law     |
| Inlet velocity                          | 35 [m/s]       |
| Inlet temperature                       | 1000 [K]       |
| Inlet electron temperature              | \( \frac{\partial T}{\partial n} = 0 \) |
| Inlet current density                   | Jn=0           |
| Current density of the cathode side wall| 5.35×10^6 [A/m^2] |
| Heat conductivity of cathode (tungsten) | 190 [W/(m·K)]  |
| Heat conductivity of anode (copper)     | 398 [W/(m·K)]  |

3. Flow Field and Hydrogen Influence

Based on the above settings, the calculated temperature of working gas is shown in Figure 2. The influence of hydrogen added to the working gas was discussed.

![Figure 2. Temperature contour of Ar and Ar+H2 working gas](image)

According to Figure 2, when hydrogen was added, temperature was nearly doubled than the working gas of pure argon. The highest temperature zone appeared near the cathode tip and the hot plasma flow dwelled mainly in the gun, while it flew outside of the gun, plasma flow was cooled down quickly by the ambient cold air, so a strong temperature gradient could be observed near the gun exit.

![Figure 3. Velocity contour of Ar and Ar+H2 working gas](image)
Adding hydrogen into argon plasma increased the enthalpy, heat and electrical conductivity, which causes the heat transfer dramatically.

According to Figure 3, the velocity of the plasma flow reached a higher value after being added hydrogen to the flow, but the gradient was also greater in the outer space. As discussed former in the paper, the heat transfer was increased by adding hydrogen, so the flow behaved more instable, which can be concluded from the Ar+H₂ flow behavior near the cathode tip.

The difference between the two working gas of temperature and velocity along the axis is showed in Figure 4.

![Figure 4. Difference between the two working gas in temperature and velocity](image)

(a) Temperature distribution along the axis  
(b) Velocity distribution along the axis

According to Figure 4, the highest temperature of the two working gas plasma flow both appeared near the cathode tip (only 2-5mm from the tip). The highest temperature changed from 6000K to 12000K after adding hydrogen to the gas. Compared to temperature, the velocity lagged behind. After being heated by the high temperature zone, the working gas expended with velocity increasing dramatically. However, after spraying into the cold air, the velocity decreased owing to the cooling down of plasma flow.

Electron number density distribution is showed in Figure 5.

![Figure 5. Electron number density distribution of atmospheric plasma flow](image)

According to Figure 5, the order of plasma number density achieved $10^{21}$. For the Ar+H₂ plasma, the electron number density increased by one order. The distribution of electron represented the ionization of plasma flow. Most of the electrons appeared in high temperature zone. But influenced by the plasma flow they moved downstream. The electron distribution was moved to the outside of the gun by the plasma flow. In the real application of plasma spraying, the powder injector is set about 9mm from the gun exit. So the injected particles would be probably charged by these electron and ions.
4. Conclusions
The Atmospheric Plasma Spray technology usually uses hydrogen as secondary working gas. The influence of hydrogen added to argon plasma was discussed in this paper. Some main conclusions were obtained.

After adding hydrogen to the argon plasma flow, the flow temperature in the gun chamber increased, but the location of high temperature zone still appeared near the cathode tip. When heading to the ambient cold air, the plasma temperature decreased. Due to the distribution of high temperature in the chamber, the working gas was heated and expanded, then reached a higher velocity.

Acknowledgments
This work was supported by Fuyang Normal University Natural Science Research Project (2016FSKJ01), Fuyang Municipal Government-Fuyang Normal University Horizontal Cooperation Scientific Research Project(XDHX2016023).

References
[1] Li H P, Pfender E 2007 Three dimensional modeling of the plasma spray process. Journal of Thermal Spray Technology.16, 245-260.
[2] Huang R, Fukanuma H, Uesugi Y, Tanaka Y 2011 Simulation of arc root fluctuation in a dc non-transferred plasma torch with three dimensional modeling. Journal of Thermal Spray Technology.21,636-643.
[3] Mauer G, Vaßen R, Stover D 2011 Plasma and particle temperature measurements in thermal spray: Approaches and applications. Journal of Thermal Spray Technology.20, 391-406.
[4] Meillot E, Guenadou D, Bourgeois C 2008 Three-dimensional and transient D.C. Plasma flow modeling. Plasma Chem Plasma Process.28, 69-84.
[5] Selvan B, Ramachandran K 2009 Comparisons between two different three-dimensional arc plasma torch simulations. Journal of Thermal Spray Technology.18, 846-857.
[6] Trelles J P, Pfender E, Heberlein J V R 2006 Multi finite element modeling of arc dynamics in a DC Plasma torch. Plasma Chem Plasma Process.26,557–575.
[7] Trelles J P, Pfender E, Heberlein J V R 2007 Modelling of the arc reattachment process in plasma torches. Journal of Physics D: Applied Physics.40,5635-5648.
[8] Huang R, Fukanuma H, Uesugi Y, Tanaka Y 2011 An improved local thermal equilibrium model of dc arc plasma torch. IEEE Transactions on Plasma Science.39,1974-1982.