Numerical simulation of multiple gas mixtures in thermal plasma using OpenFOAM

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Abstract: Gas mixtures are used to form a non-transferred arc or transferred arc in the plasma process. However, a mixture of two or more gases is not fully mixed in thermal plasmas. Thus, the diffusion rate of the gas mixture needs must be determined for modeling of thermal plasma. The combined diffusion coefficient method is applied to treat a mixture of two or three gases for various thermal plasma processes. In this study, an unsteady numerical model is developed using extended combined diffusion coefficient method predicting the distribution of the three-gas mixture. The simulation results highlight the effect of demixing in gas mixtures.

Keywords: Combined diffusion coefficients, OpenFOAM, CFD, Thermal plasmas

1. Introduction

Plasma gases such as argon, hydrogen, nitrogen, and helium are widely used to form the transferred or non-transferred arc in the plasma arc process. The plasma processes such as arc welding, plasma spraying, and plasma arc cutting, are carried out using gas mixtures to improve the efficiency. In general, a mixture of two or more gases does not fully mix. Therefore, for multiple gas mixture plasma modeling, it is necessary to determine the transport properties of the gas mixtures. In general, the combined diffusion coefficients method is utilized to model the diffusion in two- or three-gas mixture [1, 2]. A recent combined diffusion coefficients method was applied to capture the diffusion of multiple metal vapors with helium shielding gas in Tungsten inert-gas (TIG) welding of stainless steel [3, 4]. It was shown that diffusion driven by an electric field (cataphoresis) affected the diffusion of metal vapor from the weld pool to the cathode. Moreover, different diffusion behaviors were predicted for different metal vapors.

However, previous studies of three-gas mixture only considered steady-state simulations, and therefore such models cannot fully capture the unsteadiness of plasma process with larger total flow rate to total current ratios [5]. Moreover, the non-transferred arc for plasma spray is very unstable, and therefore unsteady state simulation is be required to accurately model the arc behavior.

In this paper, we present the unsteady state simulation results of free burning arcs that incorporates the combined diffusion coefficients method for a three-gas mixture. The results of the simulation are compared against those of the two-gas mixture to observe the effect of the diffusion of gas mixtures.

2. Computational model for three-gas mixture

We developed an unsteady state model of free-burning arc by using the methods proposed in [5, 6]. As shown in Fig.1, the axisymmetric computational geometry includes the cathode surface, the anode surface, and the open boundary. The arc length was 1 mm, and the simulation was performed for an arc current of 200 A. The model simultaneously solves the sets of equation for mass, momentum, energy current continuity, and mass fraction conservation for the three gases. Local thermodynamic equilibrium (LTE) was assumed, and the thermodynamic and transport properties were calculated using the methods described by Murphy [7]. However, the turbulence effect of the plasma was neglected. Moreover, the mass flux was near the electrode was neglected to treat the large mass flux due to the large difference in the temperature between the electrode and the adjacent computational cell.

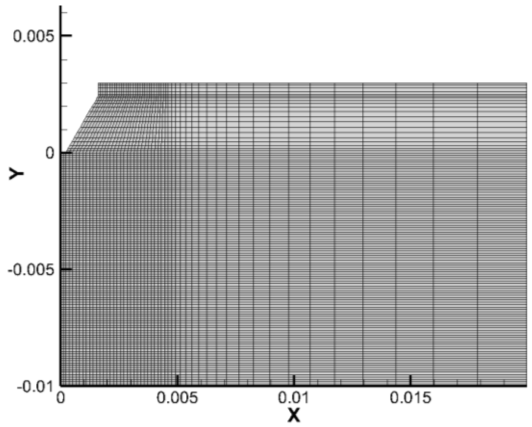

Fig. 1. Axisymmetric computational domain of multiple gas mixtures in free-burning arc.

Mathematical formulation of the proposed model

Mass conservation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \quad (1)$$

Momentum conservation

$$\frac{\partial}{\partial t}(\rho \vec{u}) + \nabla \cdot (\rho \vec{u}\vec{u}) = -\nabla p + \nabla \cdot (\mu \nabla \vec{u}) + \vec{j} \times \vec{B} \quad (2)$$

Energy conservation

$$\frac{\partial}{\partial t}(\rho h)+\nabla\cdot(\rho\vec{u}h)=\nabla\cdot\left(\frac{k}{C_p}\nabla h\right)+\frac{Dp}{Dt}+\frac{5}{2}\frac{k_b}{e}\left(\vec{j}\cdot\nabla T\right) -\nabla\cdot\left[\left(\overline{h_A}-\overline{h_C}\right)\frac{k}{c_p}\nabla\overline{Y_A}\right]-\nabla\cdot\left[\left(\overline{h_B}-\overline{h_C}\right)\frac{k}{c_p}\nabla\overline{Y_B}\right] +\vec{j}\cdot\vec{E}-Q_r \tag{3}$$

Mass fraction conservation

$$\frac{\partial}{\partial t}\left(\rho\overline{Y_A}\right)+\nabla\cdot\left(\rho\vec{u}\overline{Y_A}\right)=-\nabla\cdot\overline{\boldsymbol{J}_A} \tag{4}$$

$$\overline{\boldsymbol{J}_A}=\frac{n^2}{\rho}\overline{m_A}\,\overline{m_B}\,\overline{m_C}\left[\left(\overline{D_{AB}^x}\nabla\overline{x_B}+\overline{D_{AC}^x}\nabla\overline{x_C}\right)+\overline{D_A^P}\nabla\ln P+\overline{D_A^E}\mathbf{E}\right] -\overline{D_A^T}\nabla\ln T \tag{5}$$

$$\frac{\partial}{\partial t}\left(\rho\overline{Y_B}\right)+\nabla\cdot\left(\rho\vec{u}\overline{Y_B}\right)=-\nabla\cdot\overline{\boldsymbol{J}_B} \tag{6}$$

$$\overline{\boldsymbol{J}_B}=\frac{n^2}{\rho}\overline{m_A}\,\overline{m_B}\,\overline{m_C}\left[\left(\overline{D_{BA}^x}\nabla\overline{x_A}+\overline{D_{BC}^x}\nabla\overline{x_C}\right)+\overline{D_B^P}\nabla\ln P+\overline{D_B^E}\mathbf{E}\right] -\overline{D_B^T}\nabla\ln T \tag{7}$$

Maxwell's equations

$$\vec{j}=-\sigma\nabla\phi \tag{8}$$

$$\nabla\cdot(\sigma\nabla\phi)=0 \tag{9}$$

$$\vec{B}=\nabla\times\vec{A} \tag{10}$$

$$\nabla^2\vec{A}=-\mu_0\vec{j} \tag{11}$$

The model was implemented in OpenFOAM, which is a general purpose, open source computational fluid dynamics (CFD) package. It was developed to calculate the general fluid flow using numerous schemes and solver; however, its source code can be modified to include the plasma effect of thermal plasmas. rhopimpleFoam, which is a compressible solver, was modified to calculate the model. The algorithm of rhopimpleFoam is shown in fig 2.

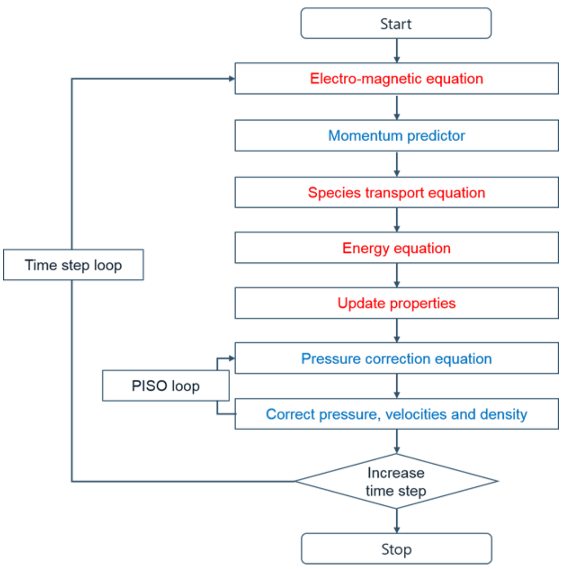

Fig. 2. Schematic of algorithm in modified rhopimpleFoam

3. Results and discussion

3.1 Distribution of mass fraction of three gases

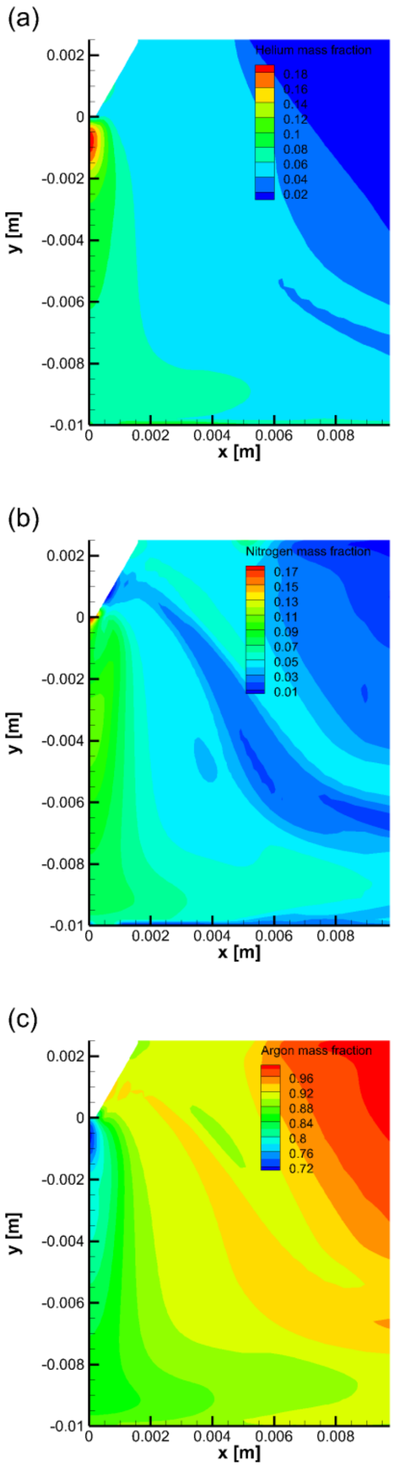

Fig. 3. Mass fraction of (a) helium, (b) nitrogen, and (c) argon at 0.015 s

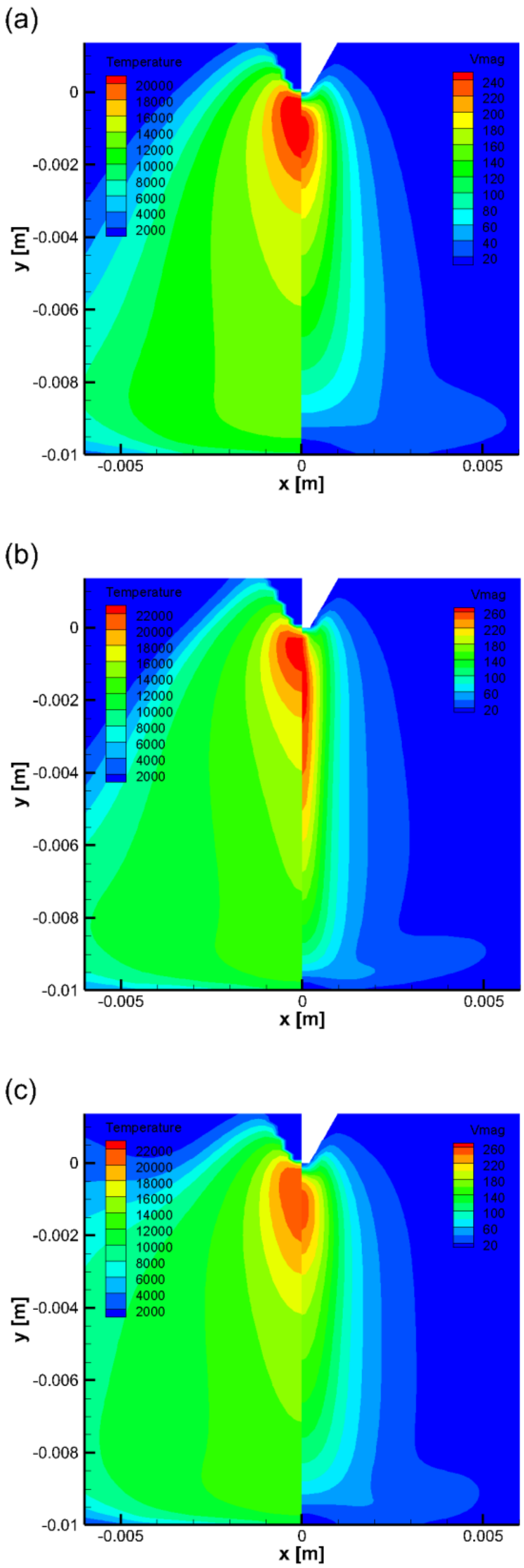

Fig. 4. Distribution of temperature(left) and velocity magnitude(right) of (a) 5% helium, 5% nitrogen, and 90% argon by mass, (b) 100% argon and (c) 5% helium and 95% argon by mass at 0.015 (s)

To investigate the effect of diffusion of gases in the mixture, helium, nitrogen, and argon were selected as the gases in the three-gas mixture. The inlet boundary condition for mass fraction of helium and nitrogen was 5% and that of argon was 90%. Figure 3 illustrates the distribution of the mass fraction of helium, nitrogen, and argon at 0.0015 s because the simulation reaches the quasi-steady state at around 0.015 s. The predicted distribution of helium mass fraction shows trends that are similar to those observed in helium-argon mixture in [6]. The concentration of helium is highest in the high temperature region at center of the arc. Moreover, the predicted distribution of nitrogen mass fraction is similar to the case of nitrogen-argon. It should be noted that the peak value of nitrogen mass fraction is not in the hottest region, but rather directly below the cathode tip. Moreover, the concentration of nitrogen near the anode is also higher than that of helium.

3.2 Comparison with other gases

Figure 4 compares the temperature and magnitude of velocity between pure argon and a mixture of 5% helium and 95% argon by mass. The maximum temperature achieved by pure argon arc was the highest, while that of the helium–argon mixture was the lowest. This can be attributed to the high ionization potential of helium, which results in a decrease in the maximum attainable temperature of the arc. Further, the velocity magnitude is largest at 281.601 m/s for pure argon because of the higher temperature.

4. Conclusion and future works

In this paper, we present the initial results of unsteady state simulation that incorporates the combined diffusion coefficient method for helium, nitrogen, and argon gas mixture. The distribution of mass fraction of each gas shows similar trends to those observed for gas mixtures such as helium–argon and nitrogen–argon. The simulation results demonstrate that the extended combined diffusion coefficient method can be applied to treat the diffusion of gas mixtures in an unsteady state model. Therefore, this approach can be applied to predict the effect of demixing of gas mixtures in plasma processes, such as plasma spray process, plasma arc cutting, or arc welding

5. References

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