Numerical Simulation of Nonequilibrium Flow in a Low-Power Hydrogen Arcjet

IEPC-2013-406

Presented at the 33rd International Electric Propulsion Conference,
The George Washington University • Washington, D.C. • USA
October 6 – 10, 2013

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Abstract: A numerical simulation has been performed of a high-velocity hydrogen plasma arc flow in a low power arcjet including a finite-rate chemical kinetic model. Electrons, ions, molecules and atoms are treated as separate species in the plasma mixture. Modeling results are found to be compared favorably with available experimental data for the arcjet thrusters. It is shown that the plasma is far from thermodynamic equilibrium in the entire arc expansion process through a nozzle. Significant temperature discrepancies between electrons and heavy species are found in the cooler outer region. The net ionization and dissociation zones are presented and discussed.

Nomenclature

\begin{align*}
B_0 & = \text{magnetic induction intensity} \\
\hat{B} & = \text{magnetic induction intensity vector} \\
D_a & = \text{ambipolar diffusion coefficient} \\
e & = \text{energy per unit mass} \\
E & = \text{electric field} \\
\hat{E} & = \text{electric field vector} \\
f & = \text{mass fraction} \\
h & = \text{enthalpy per unit mass} \\
l & = \text{total current} \\
J & = \text{current density} \\
k & = \text{chemical reaction rate coefficient} \\
k_B & = \text{Boltzmann constant} \\
L & = \text{energy loss rate} \\
\dot{m} & = \text{the mass flow rate} \\
n & = \text{number density} \\
\dot{n} & = \text{net particle production rate} \\
p & = \text{scalar pressure} \\
\dot{R} & = \text{radiative energy transfer per unit volume} \\
T & = \text{temperature} \\
u & = \text{velocity} \\
Z & = \text{thermodynamic partition functions} \\
\varepsilon_d & = \text{dissociation energy}
\end{align*}

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\[ \frac{n_{H}}{n_{e}} = \left( \frac{Z_{\text{H},e}^{3}}{Z_{\text{H},e}^{2} + Z_{\text{H},e}^{2} + Z_{\text{H},e}^{2} + Z_{\text{H},e}^{2}} \right) \exp \left( -\frac{E_{d,\text{H},e}}{k_{B}T_{h}} \right) \left( \frac{m_{H}k_{B}T_{h}}{h^{2}} \right)^{1/2} \]

Introduction

The arcjet is an electrothermal thruster which uses an arc to increase the enthalpy of the propellant which is subsequently thermodynamically expanded by a nozzle to supersonic velocities. In order to improve arcjet design, increase the efficiency and service life of arcjet thruster, there is a need to better understand the underlying physics, detailed energy balances, and transport mechanisms of these devices. Experimental techniques provide much useful empirical data for the study, but many quantities of interest are not accessible in the important regions of the thruster\(^{[1]}\). For these reasons numerical methods of solving the governing equations have become important tools for conducting arcjet research.

In recent years, we have been modeling the plasma flow and heat transfer inside the arcjet thruster based on the local thermodynamic equilibrium (LTE) assumption\(^{[2,3]}\). It has been found that in some cases, the LTE assumption can be successfully used to predict the main plasma flow features and arcjet performance. However, previous research efforts have demonstrated that both chemical and thermal processes in the arcjet are not in equilibrium due to the existence of large gradients of temperature and velocity, interactions between the electromagnetic and flow fields, and steep nonlinear variations of plasma properties associated with the spatial variation of temperature and species densities\(^{[1,4-8]}\). Investigations of nonequilibrium processes inside the arcjet thruster are necessary for a better understanding of the physical phenomena occurring there and optimization of such devices.

Modeling Approach

A. Model and Assumption

The arcjet thruster used in this simulation is a 1-kW-class radiatively cooled laboratory-type thruster, which has almost the same dimensions as the radiation-cooled arcjet thruster designed by NASA Lewis Research Center\(^{[9]}\), allowing comparison of the predictions of the model with experimental data available in the literature. Fig. 1 shows the main dimensions and the computational domain adopted in this modeling. As shown in Fig. 1, the arcjet consists of a converging-diverging nozzle through which the propellant is accelerated from subsonic to supersonic velocities. The converging and diverging sections of the nozzle are joined by a constant radius section called the constrictor, which lengthens and assists in the stabilization of the arc. Due to the axisymmetry of the thruster nozzle, only the upper half is modeled in the computation. The computational domain used in the model is denoted as B-C-I-J-F-G-H-B in Fig.1, in which C-I, I-J and J-F are respectively the inner surfaces of the convergent segment, constrictor and divergent segment of the anode/nozzle.

The main assumptions employed in the modelling study of hydrogen arcjet are as follows, (i) the arcjet is operated in the steady mode with no voltage oscillation, and the gas flow in the arcjet thruster is axisymmetric, laminar and compressible; (ii) the velocity of each the species including electrons, follows Maxwellian distributions; (iii) the thermal nonequilibrium follows a two-temperature model that separates heavy-species temperature \(T_h\), and the electron temperature \(T_e\); (iv) the plasma is optically thin; (v) electron gain energy through Joule heating from the electric field and then the energy of electrons is partially transferred to heavy species through collisions.

B. Chemical Reactions

In this study, the plasma is considered to contain electrons and heavy species of hydrogen, including molecules (\(H_2\)), atoms (\(H\)) and ions (\(H^+\)). The species productions rates, \(\dot{n}_i = m_i\dot{n}_i\), determined as a function of \(T_h\) and \(T_e\) from the assumed finite-rate chemistry processes are summarized in Table 1. The reactions chosen for this model are similar to those used in previous arcjet models\(^{[10-12]}\). For two-way reaction, the reverse reaction rates are extracted from the forward reaction and the equilibrium constants given by Eqs. (1-2).
\( \frac{n_i n^*}{n_H} = 2 \left( \frac{Z_i^*}{Z_H^{*}} \right) \exp \left( \frac{-e_i H}{k_B T_e} \right) \left( \frac{2 \pi m_e k_B T_e}{h^2} \right)^{3/2} \quad (2) \)

**Table 1. List of the processes considered in the model**

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Rate (m(^3)/s or m(^2)/s)</th>
<th>Loss rate (W/m(^2))</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 2H + M = H_2 + M )</td>
<td>( k_{f1} = \frac{1.764 \times 10^{-42}}{T_e} )</td>
<td>( L_n = (k_{e1} n_H - k_{f1} n^*_H) \rho m_c e_i H )</td>
</tr>
<tr>
<td>( H_e + e + M = H + M )</td>
<td>( k_{f2} = \frac{1.45 \times 10^{-33}}{T_e^{1.5}} )</td>
<td>( L_n = (k_{e1} n_H - k_{f2} n^*_H) \rho m_c e_i H )</td>
</tr>
<tr>
<td>( e + H_2 \to 2H + e )</td>
<td>( k_{f3} = (\sigma \nu) )</td>
<td>( L_c = 2.34 k_{e1} n_H \rho m_c e_i H )</td>
</tr>
<tr>
<td>( H^- + e \to H + h\nu )</td>
<td>( k_{f4} = \frac{6.26 \times 10^{-17}}{T_e^{0.58}} )</td>
<td>( L_n = -1.34 k_{e1} n_H \rho m_c e_i H )</td>
</tr>
<tr>
<td>( H^+ + 2e = H + e )</td>
<td>( k_{f5} = \frac{1.95 \times 10^{-20}}{T_e^{1.5}} )</td>
<td>( L_n = (k_{e1} n_H - k_{f5} n^*_H) \rho m_c e_i H )</td>
</tr>
</tbody>
</table>

**C. Governing Equations**

The field of plasma flow, temperature and concentration within the arcjet nozzle can be calculated by solving the two-dimensional continuity, momentum, energy and species conservation equations coupled with Maxwell’s equations. Chemical reaction of dissociation, ionization and recombination were taken into account in this model.

The set of governing equations in the cylindrical coordinate system can be written as follows.

\[
\frac{\partial U}{\partial t} + \frac{\partial E}{\partial z} + \frac{\partial F}{\partial r} + H = \frac{\partial E_z}{\partial z} + \frac{\partial F_r}{\partial r} + H_r + S_c + S_{EM} \quad (3)
\]

Where

\[
U = \begin{bmatrix}
\rho \\
\rho u_z \\
\rho u_r \\
\rho u_{zz} \\
\rho u_{rr} \\
\rho e_z \\
\rho e_r \\
\rho e_{zz} \\
\rho e_{rr} \\
\end{bmatrix} ;
E = \begin{bmatrix}
\rho u_z \\
\rho u_r \\
\rho u_{zz} \\
\rho u_{rr} \\
\rho e_z \\
\rho e_r \\
\rho e_{zz} \\
\rho e_{rr} \\
\end{bmatrix} ;
F = \begin{bmatrix}
\rho u_z \\
\rho u_r \\
\rho u_{zz} \\
\rho u_{rr} \\
\rho e_z \\
\rho e_r \\
\rho e_{zz} \\
\rho e_{rr} \\
\end{bmatrix} ;
H = \begin{bmatrix}
0 \\
\tau_{zz} \\
\tau_{rr} \\
\tau_{zr} \\
\end{bmatrix} ;
E_c = \begin{bmatrix}
0 \\
0 \\
\frac{\partial \rho }{\partial z} + \frac{\rho \partial u_z}{\partial z} + \frac{1}{r} \frac{\partial (r \rho u_r )}{\partial r} - \frac{\hat{q}_e}{\rho} \\
\frac{\partial \rho }{\partial r} + \frac{\rho \partial u_r }{\partial r} + \frac{1}{r} \frac{\partial (r \rho u_z )}{\partial z} + \frac{\hat{q}_e}{\rho} \\
\frac{\partial \rho e_z}{\partial z} + \frac{\rho \partial u_z e_z}{\partial z} + \frac{1}{r} \frac{\partial (r \rho u_r e_z )}{\partial r} - \frac{\hat{q}_e}{\rho} \\
\frac{\partial \rho e_r }{\partial r} + \frac{\rho \partial u_r e_r }{\partial r} + \frac{1}{r} \frac{\partial (r \rho u_z e_r )}{\partial z} - \frac{\hat{q}_e}{\rho} \\
\end{bmatrix} ;
S_c = \begin{bmatrix}
0 \\
0 \\
-J_B r \\
-J_B z \\
\end{bmatrix} ;
S_{EM} = \begin{bmatrix}
0 \\
0 \\
J_c E_r + J_r E_z \\
J_c E_z + J_r E_r \\
0 \\
0 \\
0 \\
0 \\
\end{bmatrix} ;
\]

and

\[
\rho e = \frac{p}{\gamma - 1} + \frac{1}{2} \rho (u^2 + v^2) , \quad \rho e = \frac{p}{\gamma - 1} + \frac{1}{2} \rho (u^2 + v^2) ,
\]

\[
\dot{q}_e = -D_{i1} h_m \frac{\partial n_i}{\partial z} - k_{i1} T_e \frac{\partial e_z}{\partial z} ,
\]

\[
Q_{eh} = 3 \rho \left( V_{ei} \frac{\partial e_i}{\partial z} + \frac{\partial}{\partial r} \right) \left( \frac{V_{ei}}{m_i} + \delta_e \frac{V_{ei}}{m_i} \right) k_B (T_e - T_i)
\]

The current distribution within an arcjet thruster is assumed to be two-dimensional, and the azimuthal current is expected to be zero. The current density is given by Ohm’s law.
\[ \bar{J} = \sigma (\bar{E} + \bar{u} \times \bar{B}) \]  

(4)

Rewriting Ohm’s law by making use of Maxwell’s equations for steady condition, one obtains an equation for the magnetic induction intensity in the form\(^{[13]}\):

\[ \frac{\partial}{\partial r} \left[ \frac{1}{\sigma r} \frac{\partial (rB_r)}{\partial r} \right] + \frac{\partial}{\partial z} \left[ \frac{1}{\sigma} \frac{\partial (rB_z)}{\partial z} \right] = \mu_0 \left[ \frac{\partial (u_r B_r)}{\partial r} + \frac{\partial (u_z B_z)}{\partial z} \right] \]  

(5)

In this study, the Roe scheme with MUSCL limiters, a scheme for solving hyperbolic systems of conservation equations, known for its ability to treat discontinuities, is introduced to discretize the convection terms in equation (3), and the diffusion terms are discretized by a central differencing scheme. A forth-order Runge-Kutta scheme is chosen to march forward in time. All the partial derivatives are expressed in physical space. In order to solve the governing equations from physical space into computational space is required.

D. Boundary Conditions

In this study a baseline case with mass flow rate of 14.2 mg/s and arc current of 9.8 A has been selected to show the detailed modeling results. The conditions at the inlet of the computational domain are taken to be those of a subsonic uniform flow. The boundary conditions along the centerline are set to ensure axisymmetry. At the inner wall of the arcjet nozzle, which also serves as the anode of the thruster, no slip conditions are maintained for the velocity, and the species concentrations have zero gradient. Along the inner surface of the anode, a zero gradient is imposed on the electron temperature, while the heavy-species temperature increases from the upstream boundary value of 1000 K to a maximum of 1400 K near the exit plane\(^{[10]}\). The outflow boundary conditions at the exit of the nozzle are obtained by assuming that the gradients of the variables are zero. The associated boundary conditions for the electromagnetic fields are identical to those used in Ref.\(^{[3]}\).

E. Thermodynamic and Transport Properties

We use the Chapman-Enskog theory to calculate the transport properties. In our thermodynamic and chemical nonequilibrium model, the thermodynamic and transport properties are calculated from the temperature and the composition at each position in the calculation domain for each iteration, until convergence is reached. In this study, the second-order approximations are used for viscosity and heavy species thermal conductivity. The third-order approximation is employed for electron thermal conductivity. The detailed procedure is described in Ref.\(^{[14]}\).

Results and Discussion

A. Code Validation

For the case with hydrogen as the propellant, experimental results have been reported by Cappelli and his co-workers. Our predicted results for the axial-velocity variation along the nozzle axis and the radial profiles of the axial velocity, gas temperature and electron number density at the exit plane of arcjet are thus compared with their experimental data. Fig. 2a compares the predicted radial distribution of the axial velocity at the arcjet nozzle exit with corresponding experiment results presented in\(^{[15]}\) for case with hydrogen flow rate of 13 mg/s and the electric power of 1.48 kW (arc voltage and current are 139 V and 10.3 A). It is seen that the agreement between the experimental and predicted results is fair in the central part of the jet, while the discrepancy becomes appreciable in
the fringe region, probably due to the existence of rarefaction effects near the anode-nozzle wall. Fig. 2b compares the predicted radial distribution of the electron number density at the arcjet nozzle exit with the corresponding experimental data presented in [16]. The experimental data in Fig. 2b represent the electron number density 0.4 mm downstream of the arcjet exit plane for the case with thruster power of 1.43 kW and hydrogen mass flow rate of 13 mg/s. It is seen that the peak of electron number density appear at the center and its value is approximately $10^{20}$ m$^{-3}$ and the predicted result agrees well with the experimental data.

![Figure 2](image)

**Figure 2.** Comparisons of the computed results and the experimental data concerning the axial velocity (a) and number density of electron (b) profiles at the exit plane for the thruster operating at corresponding condition.

**B. Thermal Nonequilibrium**

Typical modeling results are presented in Figs. 3-6 for the hydrogen plasma arc expansion through the arcjet nozzle for a fixed inlet mass flow rate of 14.2 mg/s and arc current of 9.8 A. Fig. 3 show the calculated fields of $T_e$ and $T_h$ in hydrogen plasma, while the electron and heavy-species temperature along the centerline and inner surface of the nozzle are shown in Figs. 4a and 4b respectively. The shadows in Figs. 4a and 4b represent the constrictor region in the arcjet nozzle. It is seen from Fig. 3 that the electron temperature is higher than the heavy species temperature throughout the whole flow field.

![Figure 3](image)

**Figure 3.** Comparison of computed electron (upper semi-plane) and heavy species (lower semi-plane) temperature distributions in hydrogen arcjet nozzle.

The central region of the arc within the constrictor is near thermal equilibrium, as shown is Fig. 4a. This is due to the high ionization fraction, which ensures efficient coupling of the electron and heavy species temperatures through Coulomb collisions between electron and ions; the primary source of energy for the heavy species is collisional energy transfer from electrons. Since most of the heating of the gas occurs inside and just beyond the constrictor, after which the flow expands and cools in the arcjet nozzle, both the electron and heavy species temperatures axially decrease from the constrictor to the exit of the nozzle, as shown in Fig. 4a. The electron and heavy species
temperature distributions along the inner surface of anode/nozzle are presented in Fig. 4b. A maximum in the electron temperature occurs at the current attachment location, where the intense heating creates a ‘hot spot’ on the anode surface. A high degree of thermal nonequilibrium is noted, with \( T_e/T_h \approx 13 \). The heavy species temperature in this region remains close to that of the anode wall sine the ionization fraction is too low to provide any significant thermal coupling to electrons. This thermal nonequilibrium largely controls the electron densities near the electrode, which in turn gives a non-zero electrical conductivity near the electrodes, even though heavy species temperature is low.

![Graph showing temperature distributions along the inner surface of anode/nozzle.](image)

**Figure 4.** Comparison of computed variations of the electron temperature, heavy species temperature and nonequilibrium parameter (\( T_e/T_h \)) along the arcjet nozzle axis (a) and the inner surface of the nozzle (b).

### C. Chemical Nonequilibrium

As stated above, the five reactions involved in this kinetic model are listed in Table 1, which also includes the reaction heat. The ionization fraction contours, *i.e.*, those of the ratio of the electron number density to the heavy species number density, are shown in Fig. 5a. It is interesting to find that the ionization degree in arc core presented here is quite low, only 43%, which is different from the value more than 70% calculated in a state of equilibrium condition. It is found that the computed axial velocity at the constrictor exit center is more than 10 000 m/s, while the length of the constrictor is 0.25 mm. Thus one obtain a fluid residence time in the constrictor of order 0.025 μs, which is comparable with the ionization relaxation time of hydrogen. The electric field rapidly heats the electrons, while the degree of ionization usually lags behind the values that would correspond to the rising electron temperature\[^{[17]}\]. The computed mass fraction contours of hydrogen atoms within the arcjet nozzle are shown in Fig. 5b. It is seen that the concentration of hydrogen atoms are mainly on the center line of the arcjet and the dissociation fraction is small in the cold flow area between axis and the anode. It is found from Figs. 5a and 5b that the hydrogen molecules appear in most of the flow region instead of the hydrogen atoms or ions.

![Graph showing computed ionization and dissociation fraction contours within the arcjet nozzle.](image)

**Figure 5.** Computed ionization (a) and dissociation fraction (b) contours within the arcjet nozzle.
Fig. 6 shows a contour plot of the net production rate of electrons/ions and atoms within arcjet thruster. It can be noted from the upper semi-plane that the region of net ionization covers not only the core of the arc in the constrictor, but also the upstream of the region near the anode/nozzle wall. In these two regions the temperature of electron is high enough for the ionization reaction. While the electron used for maintaining the arc in the cold flow region is derived from diffusion. It is also shown that hydrogen molecules dissociate in most part of the flow field. The recombination zone on the downstream of the center is caused by the large number of the hydrogen atoms delivered from the upstream without recombining in time. And the negative value of net hydrogen atoms production rate occurs in the inflow and downstream of the cold flow region is caused by the low-temperature of both electron and heavy species.

![Figure 6. Dissociation and ionization contours within arcjet thruster.](image-url)

**Conclusion**

A self-consistent nonequilibrium plasma model has been carried out to study the nonequilibrium phenomenon within the arcjet with hydrogen as the propellant. Modeling results are compared with available experimental data and found to compare favorably for the arcjet thrusters. Numerical results show that considerable thermal nonequilibrium exists in the entire arc expansion process through a nozzle especially in the near anode/nozzle wall region. In addition, the chemical reaction including the dissociation, ionization and recombination process, are used to take the chemical nonequilibrium effects into account, and the calculations show clearly that strong departures from dissociation and ionization equilibrium exist in the arcjet thrusters.

**Acknowledgments**

This work was supported by the National Natural Science Foundation of China. (Grant Nos. 11275021, 11072020, 50836007)

**References**


