Plasma expansion in the preshock region

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The supersonic expansion of an underexpanding argon plasma from a high density arc source with small dimensions into a low-pressure vessel with large dimensions is studied by an extended one-dimensional nonlocal thermal equilibrium fluid model, called SPIRIT. In an expanding plasma the velocity increases and the pressure, the density, and the temperatures decrease severely. In this article the virtual source model is discussed first, which is a model describing the expanding plasma as originating from a virtual source. The virtual source model includes some viscosity and heat transport in simplified form, but most of the viscosity and heat transport contributions are neglected. The SPIRIT code includes the full energy and momentum balances. The inclusion of viscosity and heat sources may lead to deviations from an adiabatic and/or isentropic expansion. The SPIRIT code can analyze the deviations. When deviations are small, the isentropic expressions from gas dynamics can be used to model expanding plasma too. Model outcomes are compared with experimental data. © 2001 American Institute of Physics. [DOI: 10.1063/1.1390309]

I. SETUP

Expanding plasmas admixed with deposition gases are used for the deposition of thin layers and to modify surface layers. To optimize these processes a high source strength, knowledge of how to control the expanding flow, and information about the mixing of the deposition gas with the carrier gas is needed. Therefore it is necessary to have basic knowledge of the expanding argon plasma investigated here.

The argon plasma source considered is a dc wall-stabilized thermal cascaded arc. The power dissipation is typically of the order of 5 kW, using an arc current of 50 A. The cascaded arc produces a thermal argon plasma at sub-atmospheric pressure, characterized by an electron temperature of 1 eV and high electron densities of \(10^{22} - 10^{23} \text{ m}^{-3}\). Flows are typically between 10 and 150 sccs \(= 2.5 \times 10^{19} \text{ particles/s}\). The arc channel in this study has a constant diameter of 4 mm.

The expansion chamber is a low pressure vessel at a varying downstream pressure of 20 Pa–10 kPa. The dimensions of the vessel are 1 m diameter and 1.5 m length. The plasma is said to be “under-expanded” because the pressure in the exit plane is higher than the background pressure. The expansion occurs supersonically due to the large pressure difference between the plasma source and the background gas in the expansion chamber. The setup is shown in Fig. 1.

II. INTRODUCTION

A. The virtual source model

To describe the so-called preexpansion, i.e., the expansion from about one arc diameter from the expansion inlet to about a few mean free paths before the normal shock, we refer to the “virtual source” model of Ashkenas and Sherman. This model assumes that the plasma diverges from a virtual point just after the expansion inlet. The flow lines starting in this virtual point form a fan. The flow lines of the fan of this expansion are assumed to be straight. An advantage of the virtual source model is its rather simple form. The virtual source model predicts the decrease in densities as measured by Refs. 6–15. The measured densities fall with the square root of the distance from the expansion inlet.

In Fig. 2 a schematic picture of the “virtual source” model is shown. In the cascaded arc channel the flow is straight, i.e., the flow lines are parallel, and becomes sonic at the arc outlet (the expansion inlet). At the start of the expansion there is suddenly no boundary anymore but only a background gas at an extremely low pressure. The plasma flow diverges forming a fan. The plasma is accelerated by the large difference in pressure along a distance of one or two arc channel diameters. Afterwards the velocity along each flow line remains almost constant. Also the directions of the flow lines remain constant. This pattern remains “frozen” until the normal shock at the end of the preexpansion is reached.

Experiments of Ref. 4 show that the plasma expands supersonically and that in the expanding plasma a stationary
normal shock occurs at a relatively short distance from the arc outlet. Observations and modeling on argon plasmas by van de Sanden\textsuperscript{16} indicate the usefulness of the virtual source model to our specific case.

B. The position of the normal shock

Several authors have determined the position of the stationary shock front after the supersonic expansion of a free jet as a function of the ratio of the stagnation pressure at the outlet, $p_e$, and the background pressure, $p_b$. Ashkenas \textit{et al.}\textsuperscript{5} obtained an empirical relation between the position $d_i$ and $p_e/p_b$:

$$d_i = 2rC \sqrt{\frac{p_e}{p_b}} \quad (1)$$

where $r$ is the radius of the inlet of the expansion and $C$ equals 0.67 and is independent of the isentropic exponent $\gamma$. This same relation has been derived by Young\textsuperscript{17} using the entropy and pressure balances. Young finds a somewhat higher constant which depends slightly on $\gamma$: $C\approx0.76$ for $\gamma=5/3$, and $C\approx0.67$ for $\gamma=1.2$.

C. The cross section of the normal shock

In this section we consider within the system of the cascaded arc, the expansion, the shocks, and the background gas of the following two control volumes. The boundaries of the first control volume (i.e., the preexpansion) are the arc outlet, the jet boundaries, and a virtual plane just in front of the Mach disk shock. The second control volume contains the normal Mach disk shock. To simplify matters we use the following subscripts: 1 for the arc outlet, 2 for the virtual plane just before the shock, and 3 just for after the shock.

The continuity equation gives

$$A_1\rho_1u_1 = A_2\rho_2u_2 = A_3\rho_3u_3 \quad (2)$$

with $A$ the cross section, $\rho$ the mass density, and $u$ the axial velocity. The velocity $u$ is perpendicular to the cross section, which may be curved. It is assumed that the velocity $u$ is the same along every streamline in the expansion. This means that in this approximation no radial velocity profile is assumed.

We will assume that viscous effects can be neglected before the shock, since it plays only a significant role in the formation of shocks. Euler’s momentum law, i.e., no viscosity influence before the shock, reads

$$\frac{dp}{\rho ds} + \frac{dv}{ds} = 0 \quad (3)$$

with $ds$ an infinitely small part of the considered streamline. Integrated over a streamline (from position 1 to 2, using the isentropic relation between $p$ and $\rho$), expression (3) yields

$$\frac{u_2^2}{2} - \frac{u_1^2}{2} + \frac{\gamma-1}{\gamma-1} p_1 \left[ \frac{p_2}{p_1} \right]^{(\gamma-1)/\gamma} - 1 = 0 \quad (4)$$

The Rankine–Hugoniot shock relation gives

$$\rho_2u_2^2 + p_2 = \rho_3u_3^2 + p_3 \quad (5)$$

We will further use the velocity of sound, $c$, for a calorically perfect flow defined as

$$c = \sqrt{\frac{\gamma p}{\rho}} = \sqrt{\gamma RT_p} \quad (6)$$

with $T_p$ the plasma temperature (i.e., the heavy particle temperature plus the ionization degree times the electron temperature).

Next we will consider the two control volumes separately to find some rough estimates. Simplifying with respect to the preexpansion control volume, using continuity

$$u_2 = \frac{A_1\rho_1}{A_2\rho_2} u_1 \quad (7)$$

yields using the integrated Euler expression (4) ($p_1 \gg p_2$, i.e., a “deep” underexpanding plasma)

$$\frac{u_2^2}{2} \left[ \frac{p_1A_1}{\rho_2A_2} \right]^{2} - 1 = \frac{\gamma}{\gamma-1} \frac{p_1}{\rho_1} \quad (8)$$

Rewriting terms and using the definitions of the speed of sound and the Mach number, we get

$$\frac{A_1}{A_2} = \frac{\rho_2}{\rho_1} \left[ \frac{2}{(\gamma-1)M_1^2} + 1 \right]^{1/2} \quad (9)$$

We can use expression (9) to calculate the cross-sectional area of the Mach disk normal shock. Since in our case $M_1 \approx 1$, we get
we chose the radius of the expansion \( R \) in Ref. 21 and chapter 3 of Ref. 20.

The extended one-dimensional model SPIRIT is able to verify if the plasma expands isentropically.

In this section expansion simulation results from the extended one-dimensional model SPIRIT (see chapter 7 of Ref. 20) are compared with experimental data obtained by van de Sanden\textsuperscript{16} and Meulenbroeks.\textsuperscript{24,25} Since SPIRIT includes the full electron and heavy particle energy balances, SPIRIT is able to verify if the plasma expands isentropically.

In Refs. 20 and 21 the isentropic exponent for plasmas has been derived. The isentropic exponent was found considering the thermodynamics of plasmas. In these references, there was not need to consider steady or flowing plasmas in particular, however, it is not clear if the same isentropic ex-

\[
\frac{A_1}{A_2} = \frac{\rho_2}{\rho_1} \sqrt{\frac{\gamma+1}{\gamma-1} \left( \frac{p_2}{p_1} \right)^{1/\gamma} \sqrt{\frac{\gamma+1}{\gamma-1}}}. \tag{10}
\]

Note that, since \( M_1=1 \) and \( \gamma=1.2 \),

\[
A_1 \approx \sqrt{11} \frac{\rho_2}{\rho_1} = \sqrt{11} \left( \frac{p_2}{p_1} \right)^{1/\gamma} \tag{11}
\]

and

\[
\frac{u_1}{u_2} \approx \frac{1}{\sqrt{11}}, \tag{12}
\]

which means that at the end of the expansion of the plasma \( p_2 \approx R_2^{-2} \) \( (R_2 \) is the radius of the normal shock) (see also Ref. 18) and that the increase in velocity is about 3.3 times.

We conclude, taking densities from Ref. 16, that the ratio of the cross sections can easily be a factor of 100–1000.

For the shock, we use the continuity expression (2) and the Rankine–Hugoniot jump conditions (5) taking \( A_3 = A_2 \).

Using the definition of the speed of sound, we find an adiabatic expression

\[
u_2 = \frac{\rho_3}{\rho_2} \frac{M_2}{M_3} \sqrt{\frac{T_{p,2}}{T_{p,3}}} = \frac{M_2}{M_3} \sqrt{\frac{2 + 2M_2^2}{2 + 2M_2^2}} \tag{13}
\]

Note that now, using \( M_3 \approx 1 \) (Ref. 19) and \( \gamma=1.2 \),

\[
u_2 = \frac{M_2}{M_3} \frac{2 + 0.2M_2^2}{2.2} \tag{14}
\]

Finally we can relate the parameters after the shock to the inlet conditions. This gives approximately

\[
u_1 = \frac{M_2}{M_3} \sqrt{\frac{2 + 0.2M_2^2}{24}} \tag{15}
\]

We get using \( A_3 = A_2 \),

\[
\frac{A_1}{A_2} = \frac{\rho_3}{\rho_1} \frac{M_3}{M_2} \sqrt{\frac{24}{2 + 0.2M_2^2}} \tag{16}
\]

which means that \( u_3 < u_1 \) for shocks with a Mach number higher than 2.5 (note that always \( u_3 < u_2 \)). As before we find \( \rho_2 \approx R_2^{-2} \), in agreement with Ref. 18, and the cross section of the normal shock is bigger when the shock is stronger (i.e., \( M_2 \) is larger).

\[
\frac{R_2}{R_0} = 1 + \frac{z^2}{z_0^2} \tag{17}
\]

where \( z \) is the \( z \) coordinate, \( R_0 \) is the radius of the plasma source channel, and \( z_0 \) is the virtual source location. The location of the virtual source is set equal to the radius of the plasma source channel \( R_0 = z_0 \) (Ref. 16) and is outside the plasma source channel. For \( R_0 \approx z_0 \) expression (17) becomes

\[
R = \sqrt{R_0^2 + z^2} \tag{18}
\]

which is, after bout one diameter after the start of the expansion, a 45° expanding plasma. This choice is in agreement with the virtual source model, while it permits a continuous flow from the source channel into the expansion. From conservation of flow and expression (17)

\[
\rho u = \frac{\rho_{\text{inlet}} u_{\text{inlet}}}{1 + \frac{z}{z_0}} \tag{19}
\]

where \( \rho \) is the mass density and \( u \) is the velocity. The flow at the inlet of the expansion (at \( z = 0 \)) is equal to \( \rho_{\text{inlet}} u_{\text{inlet}} \pi R_0^2 \).

The expansion radius is depicted in Fig. 3. Note that the geometry in Fig. 3 is almost the straight expansion from a virtual source with an expansion angle of 45° as used by Refs. 16 and 22–25. The length of the expansion is set equal to the position of the normal shock. The position of the normal shock is taken from expression (1) in Sec. II.B.

In the next section expansion results for a “deep” under-expanding argon plasma are compared with experimental data from Refs. 16 and 26–28. Simulation results are obtained including axial thermal conductivity. To compare our findings with gas dynamics literature,\textsuperscript{19,29–32} an isentropic argon gas expansion is included.

D. The SPIRIT model

In this section we will show the results of the argon plasma expansion from a straight arc with a diameter of 4 mm. The extended one-dimensional nonlocal thermal equilibrium hydrodynamical model SPIRIT (see chapter 7 of Ref. 20) is used in which the isentropic exponent for argon plasmas is calculated to conform to the expressions as reported in Ref. 21 and chapter 3 of Ref. 20.

To determine the geometry of the expansion boundary we chose the radius of the expansion \( R \) equal to

\[
\frac{R^2}{R_0^2} = 1 + \frac{z^2}{z_0^2} \tag{17}
\]

where \( z \) is the \( z \) coordinate, \( R_0 \) is the radius of the plasma source channel, and \( z_0 \) is the virtual source location. The location of the virtual source is set equal to the radius of the plasma source channel \( R_0 = z_0 \) (Ref. 16) and is outside the plasma source channel. For \( R_0 \approx z_0 \) expression (17) becomes

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where \( \rho \) is the mass density and \( u \) is the velocity. The flow at the inlet of the expansion (at \( z = 0 \)) is equal to \( \rho_{\text{inlet}} u_{\text{inlet}} \pi R_0^2 \).

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III. RESULTS FROM THE HYDRODYNAMIC MODEL SPIRIT

In this section expansion simulation results from the extended one-dimensional model SPIRIT (see chapter 7 of Ref. 20) are compared with experimental data obtained by van de Sanden\textsuperscript{16} and Meulenbroeks.\textsuperscript{24,25} Since SPIRIT includes the full electron and heavy particle energy balances, SPIRIT is able to verify if the plasma expands isentropically.

In Refs. 20 and 21 the isentropic exponent for plasmas has been derived. The isentropic exponent was found considering the thermodynamics of plasmas. In these references, there was not need to consider steady or flowing plasmas in particular, however, it is not clear if the same isentropic ex-
ponent is found under conditions of extremely fast flowing plasmas, i.e., under supersonic conditions. Here we will verify if the same isentropic number of 1.2 is found under supersonic plasma conditions.

In the case of a gas expansion, the considered underexpansion is almost isentropic. Therefore, since the isentropic relation between the argon atom density \( n \) and the temperature of the expanding gas \( T \) holds,

\[
\frac{n_{\text{gas}}}{T_{\text{gas}}^{\gamma_{\text{gas}}-1}} = \text{constant,}
\]

an isentropic exponent \( \gamma_{\text{gas}} \) of \( 5/3 \) should be found in the case of the expanding gas. In the case of an argon plasma expansion, we can verify if the plasma is isentropic by plotting the relation

\[
\frac{n_{\text{plasma}}}{T_{\text{plasma}}^{\gamma_{\text{plasma}}-1}} = \text{constant}
\]

and verify if an isentropic exponent \( \gamma_{\text{plasma}} \) of 1.2 is found.

Table I shows the inlet and jet boundary conditions as used in the simulations for the expansions. The flow (about 200 sccs) is calculated from these values. Note that by choosing the jet boundary temperature (and the radial temperature profile) in fact the radial heat flux is determined.

From the background pressure (40 Pa), the inlet flow, and inlet pressure (20 kPa) the expansion length is determined using the expression in Sec. II B. The expansion length is about 100 mm, similar to that reported by Ref. 16.

Next, the densities and the temperatures, for which experimental data are available, will be considered first before the flow parameters (the Mach number, the velocity, and the pressure). For the velocity, measured values from a comparable situation are included (data from exactly the same experimental conditions are not available).

In Fig. 4 the argon atom density in the expansion is shown. The diamonds in the figure are experimental values taken from Ref. 16. The crosses (¡) are the modeling results using SPIRIT. In agreement with Refs. 5–15 the atom density decreases with the square of the axial coordinate.

In Sec. II C we reported how the ratio of the cross section of the expansion inlet and the cross section of the normal shock is related to the ratio of the mass density at the inlet of the expansion and the mass density at the end of the preexpansion, expression (11). According to Fig. 3 the increase in cross section over the expansion is about 2500, and according to Fig. 4 the (mass) density falls almost four orders, similar to that estimated using expression (11).

In Fig. 4 the electron density in the expansion is also shown. The circles are experimental values taken from Ref. 16 and the crosses (x) are the modeling result using SPIRIT. The electron density also decreases with the square of the axial coordinate.

In Fig. 4 the experimental values and the modeling results show the same decrease. As indicated by the SPIRIT model with which the causes of the decrease are examined, the decrease in densities is mainly a result of the increase in cross section of the expanding plasma.

In Fig. 5 the average electron temperature and the average heavy particle temperature in the expansion are shown. Due to the increase in cross section both temperatures decreases fast. The decrease in heavy particle temperature is deeper than the decrease in electron temperature. Close to the start of the expansion the plasma is close to in local thermal equilibrium.

Comparing the modeled electron temperature with the measured electron temperature, it is found that the SPIRIT model underestimates the electron temperature in the expansion. Considering the heavy particle temperature, it is found that the SPIRIT model overestimates the measured heavy particle temperature in the early expansion and underestimates the measured heavy particle temperature later. It should, however, be noted that the obtained experimental values from Refs. 26 and 27 are data from an argon expansion in which hydrogen is added. The expansion has a somewhat different structure from that of pure argon gas.

In Fig. 5 the average electron temperature and the average heavy particle temperature in the expanding argon plasma.
what higher background pressure and a different arc outlet nozzle is used (i.e., the nozzle has a 45° opening angle). Due to those differences absolute values cannot be compared, but the trend behavior should be similar. Further, the normal shock location in the experiment of Refs. 26 and 27 occurs somewhat earlier than in the model using Ashkenas. In contrast to the heavy particle temperature, the measured values for the electron temperature are taken from Ref. 16 whose experimental conditions are similar to the ones used in the SPIRIT model. The SPIRIT model therefore represents the measured electron temperature better than the measured heavy particles temperature.

According to Fig. 6 recombination is mainly active close to the expansion inlet. Recombination becomes important due to the low expansion temperatures but is reduced in effectiveness by the low electron density. Therefore recombination is more effective at the start of the expansion where temperatures are already low but the electron density is still high.

In Fig. 7 we show the Mach numbers as modeled for the expansion. As can be seen from this picture, the Mach number increases when the so-called strength of the expansion, this is the cross section, increases.

In Sec. II C, expression (16), we reported how the Mach number at the shock, \( M_{\text{shock}} \), and the cross section of the normal shock are related. We could estimate \( M_{\text{shock}} \) from the ratio of the cross section at the expansion inlet and the cross section of the normal shock, and the ratio of the mass density at the normal shock and the mass density behind the normal shock. In the cases reported here the cross section ratio is about 2500 and the jump in density over the normal shock is about two orders (background densities are typically \( \times 10^{21} \) taken from Ref. 33). This implies strong shocks with high Mach numbers higher than 10 \( M_3 < 1 \) (Ref. 19).

The velocity (Fig. 8) and the pressure (Fig. 9) show the same response to a change in boundary jet cross section as the Mach number, Fig. 7. An increase in start cross section shows a relatively large increase in velocity and a relatively large decrease in pressure. The velocity in the late preexpansion does not change much anymore. The velocity at the normal shock is roughly 2.5 times higher than the expansion inlet velocity, which is 35% lower than according to expression (12) in Sec. II C. The measurements show a decrease in velocity at the late preexpansion. These measurement values are in fact shock values measured inside and after the normal shock. In case of the measurements the shock is closer to the expansion inlet due to the fact that these values are obtained with a different anode configuration, i.e., end of the arc channel. The diameter of the arc channel increases already inside the anode before the modeled expansion starts.

Comparing the modeled velocity with the measured velocity,26–28 it is found that the SPIRIT model underestimates the electron velocity in the expansion. As noted before considering the heavy particle temperature, the obtained experimental values from Refs. 26–28 are data from an argon expansion to which hydrogen is added, the expansion in which the measurement data were obtained has a somewhat higher background pressure, and a different arc outlet nozzle is used. As before, due to those differences absolute values cannot be compared, but the trend behavior should be similar. We just mentioned that the velocity in the late preexpansion does not change much anymore, something the measurements agree upon.

To simulate with SPIRIT the measured velocities of Refs. 27 and 28 a full slip condition is used. A no-slip condition at
the jet boundary caused the model not to converge anymore. This is in agreement with the virtual source model, where the outer flow line is considered as the jet boundary. Therefore the jet boundary is not determined by the location where the velocity equals zero. However, the jet boundary is the envelope for the plasma flux.

IV. DISCUSSION

A. Isentropic flow

Modeling expansions, it is often assumed that the flow is isentropic which simplifies the calculations severely. The SPIRIT model allows us to examine the isentropy conditions more closely, since it includes the sources for anisotropy, i.e., viscosity and heat sources. In the plasma expansion as reported in this article, it is noticed that the contribution of the viscosity terms and the heat conductivity are negligible. This means viscosity and heat conduction are unimportant as a source for anisentropy for our expanding plasma. Taking into account that the isentropic exponent of an expanding plasma differs from the corresponding expanding gas (see Refs. 20 and 21), it is possible that the supersonic plasma expands isentropically with the isentropic exponent of plasma (1.2).

An isentropic gas expansion is modeled and compared with the argon plasma expansion to verify the behavior of isentropic expansions. From Refs. 20, 34, and 35 it is suggested that the flow behavior (e.g., the Mach number) of expanding plasmas differs from expanding gases (e.g., the sonic position is found downstream of the throat in the case of geometrically pinched plasma flows). Note that the viscosity terms and heat conductivity cause the difference between the expansion of an argon plasma and that of an isentropic argon gas. We just saw that viscosity and (external) heat sources are also the causes of anisentropy. We stated that these contributions can be neglected in the plasma expansion. Therefore if the plasma and the corresponding gas are (quasi-) isentropic (i.e., viscosity and heat conductivity are negligible), then their behavior is expected to be the same except for the value of the isentropic exponent.

From the slope of the logarithm of the relative heavy particle temperature versus the logarithm of the relative atom density ($n_H$), and from the slope of the logarithm of the relative electron temperature versus the logarithm of the relative atom density, the isentropic exponent can be determined using the relations (20) and (21).

Figure 10 indicates that the relation between the electron temperature and the atom density in the expanding plasma conforms to the isentropic relations from gas dynamics\textsuperscript{19,29} with the corresponding plasma isentropic exponent, equal to 1.3 to 1.4, which is somewhat higher than the isentropic exponent, 1.2, from Refs. 20 and 21. Nevertheless, the isentropic exponent is roughly a constant. Note that the isentropic relation does not hold at the start of the expansion.

Figure 10 shows that the relation between the heavy particle temperature and the atom density in the expanding plasma also conforms to the isentropic relations from gas dynamics. Again, roughly spoken, a constant exponent is found. However, the value of the isentropic exponent, 1.5, is closer to the corresponding gas, i.e., roughly 5/3.
van de Sanden\textsuperscript{16} axial heat conduction is important by which the decrease in temperature will be diminished.

When the electron temperature and the heavy particle temperature in the expanding argon plasma are compared with calculations in which axial heat conductivity is not included, it is found that axial heat conductivity decreases the temperature in the start of the expansion and increases the plasma temperature close to the normal shock, which is in agreement with van de Sanden. However, according to our calculations the difference is negligible.

V. CONCLUSIONS

An expanding argon plasma flow has been modeled using the one-dimensional hydrodynamical model SPIRIT.

For an argon plasma created in a 4 mm diameter straight cascaded arc, we showed typical results for the expansion. The velocity and the Mach number increase, while the pressure, the densities, and the electron and the heavy particle temperatures decrease due to the increase in expansion cross section. With respect to deviations from local thermal equilibrium, recombination occurs mainly at the start of the expansion and the plasma deviates moderately from temperature equilibrium in the late expansion.

The trend values we found are roughly in agreement with results reported by Refs. 15, 22–25, 36, and 37. Important is the result that, in the expansion, the plasma densities are inversely related to the square of the axial coordinate. This result can be used to estimate globally the change in the plasma parameters over the expansion.

Further, the “deep” underexpanding plasma expands isentropically with the isentropic exponent of plasmas from Refs. 20 and 21 for the electrons, and with the isentropic exponent of the corresponding gas for the atoms. It is discussed that the expanding plasma might be “disconnected.”

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28. S. Mazouffre (private communication).