Numerical Calculations on Reflection Processes of Ionizing Shocks on the End Wall of a Shock Tube

Yasunari Takano and Teruaki Akamatsu
Kyoto University, Kyoto, Japan

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Numerical calculations have been made about shock reflection processes in ionizing argon on the end wall of a shock tube. The two-step Lax-Wendroff scheme was employed to solve time-dependent one-dimensional inviscid flow problems for ionizing gases. Complicated flowfields were found to occur due to interactions between ionization relaxation processes and reflected shocks. Calculations were performed for three cases: incident-shock Mach number $M_s = 16$ and initial pressure $p_1 = 1$ torr; $M_s = 14$ and $p_1 = 3$ torr; $M_s = 12$ and $p_1 = 5$ torr.

1. Introduction

Shock tube apparatuses are often utilized for the investigation of high-temperature gasdynamics, and thermodynamic- and transport-properties. Hot stagnant ionized gases behind reflected shocks at the end wall of a shock tube have been used for experimental studies of the thermal conductivity, the heat transfer rate on the end wall, the ionization relaxation time and the development of the end wall boundary layer. Therefore, it is important to elucidate the situation in the reflected-shock flowfields. Several experimental investigations have indicated that these gas regions are complicated due to the interactions between ionization relaxation processes and reflected shocks. Smith made measurements of the pressure-history at the end wall of a shock tube. He proposed a distance-time diagram of the reflected-shock flowfield in ionizing xenon, assuming simple models, in order to explain his experimental results. Kuiper and Bershader visualized the flowfields behind reflected shocks in ionizing argon by use of streak interferometry.

Numerical calculations of reflected-shock flowfields in relaxing gases have been performed for vibrational- and dissociative-gases. But, to our knowledge, no numerical calculation has been carried out of the reflection processes in an ionizing gas in which more drastic changes occur than in chemically reacting gases. The present paper deals with numerical calculations on reflected-shock flowfields in ionizing argon gases. A finite difference method is employed to solve the time-dependent, one-dimensional inviscid flow problems for ionizing gases.

There are several phenomena affecting the reflected-shock flowfields, beside ionization relaxation processes. Briefly, we shall refer to these effects in the following. The unsteady thermal boundary layer forms on the end wall as a result of wall cooling. It gives rise to a negative displacement and reduces the reflected shock. As is well-known, the side-wall boundary layer developed behind an incident shock bifurcates reflected shocks in a polyatomic gas, but not in a monatomic gas. However the bifurcation of reflected shock in ionizing argon was reported to result from the onset of ionization behind the incident shock. The radiation cooling, after ionization equilibration, also reduces the enthalpy of the ionized gas.

The above-mentioned phenomena provide their own problems to be studied. In the present paper, the effect of ionization relaxation processes on a reflected-shock flowfield is investigated in detail.

2. Numerical Analysis

2.1. Basic Equations

A schematic distance-time diagram is shown in Fig. 1, where $x$ is the distance from the end wall of a shock tube and $t$ is the time after reflection of an incident shock. The basic equations used in the present study are time-dependent one-dimensional conservation equations for ionized and thermally nonequilibrium inviscid gases:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0, \quad (1)$$

$$\frac{\partial (\rho u)}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} = 0, \quad (2)$$
\[
\frac{\partial}{\partial t} \left[ \rho \left( e + \frac{u^2}{2} \right) \right] + \frac{\partial}{\partial x} \left[ \rho u \left( e + \frac{u^2}{2} + p \right) \right] = 0 \quad (3)
\]

where \( \rho, u, p \) and \( e \) are the density, the velocity, the pressure and the energy. The equations of state for ionized monatomic gases are

\[
p = \rho (k/m) (T + cT_e), \quad (4)
\]

\[
e = 3p/2 \rho + c(E_i/mh) \quad (5)
\]

where \( T, T_e \) and \( c \) are the temperature of heavy particle gas, the electron temperature and the degree of ionization respectively, and \( k, mh \) and \( E_i \) are the Boltzmann constant, the mass of a heavy particle and the ionization energy.

The electron conservation equation \(^{10}\) is

\[
\frac{\partial n_e}{\partial t} + \frac{\partial (n_e u)}{\partial x} = \dot{n}_e \quad (6)
\]

where \( n_e \) is the number density of electron and \( \dot{n}_e \) is the electron production rate. Equation (6) can be written in term of the degree of ionization as follows

\[
\frac{\partial (\rho \dot{c})}{\partial t} + \frac{\partial (\rho \dot{c} u)}{\partial x} = \dot{q} \dot{c} \quad (7)
\]

where \( \dot{c} \) is the production rate of the degree of ionization.

The energy conservation equation of electron \(^{10}\) is

\[
\frac{\partial}{\partial t} \left( \frac{3}{2} n_e kT_e \right) + \frac{\partial}{\partial x} \left( \frac{3}{2} n_e kT_e u \right) + n_e kT_e \frac{\partial u}{\partial x} = 3 \frac{m_e}{mh} n_e k(T - T_e) v_{eh} - E_i(\dot{n}_e) e \quad (8)
\]

where \( m_e \) is the mass of an electron, \( v_{eh} \) is the collision frequency between electron and heavy particles, and \( (\dot{n}_e) e \) is the electron production rate due to atom-electron inelastic collisions. It is convenient for the numerical analysis to assume the electron gas in a local steady state: each term on the left-hand side of Eq. (8) is much smaller than either of the terms on the right-hand side. Then, the differential equation (8) reduces to such an algebraic equation as

\[
T - T_e = \frac{1}{3 \left( \frac{m_e}{mh} \right) v_{eh}} T_{ion} \quad (9)
\]

where \( T_{ion} = E_i/k \) is the characteristic temperature of ionization. The local steady state approximation is known to be valid in almost all the part of the relaxation region except the ionization initiation zone immediately behind an incident shock \(^{11}\).

The surface of the shock tube end wall located at \( x = 0 \), is assumed to be impermeable and thermally insulated. This condition means that two identical shocks collide each other at the symmetric plane \( (x = 0) \). After all, the differential equations (1), (2), (3) and (6) are to be solved with the algebraic relations of (4), (5) and (9). The initial conditions can be given by the profiles of ionization relaxation behind the incident shock propagating into the initial stationary region.

### 2.2. Ionization Production Rates and Collision Frequencies

In this section, we shall write down the formulas of ionization production rates and collision frequencies for argon plasma given by Hoffert and Lien \(^{11}\).

The ionization reaction consists of two processes. One is the production due to atom-atom inelastic collisions:

\[
\dot{c}_a = (1 - c) \left( \frac{q}{mh} \right)^2 k_{ra}(T) \frac{c_{eq}^2(T) - c^2}{1 - c_{eq}^2(T)} \quad (10)
\]

where \( c \) is the production rate of the degree of ionization.

Therefore, the net rate of the degree of ionization is

\[
\dot{c} = \dot{c}_a + \dot{c}_e \quad (12)
\]

The equilibrium degrees of ionization are written as

\[
c_{eq}(T_M) = \left[ 1 + (1 + c) \left( \frac{1 + c}{m_e K_{eq}(T_M)} \right) \right]^{-1/2} \quad (13)
\]

where \( K_{eq}(T_M) \) is the equilibrium constant \( (T_M = T \) or \( T_e) \):

\[
K_{eq}(T_M) = \frac{2Z_i}{Z_a} \left( \frac{2 \pi m_e kT_M}{k^2} \right)^{3/2} \exp \left( - \frac{T_{ion}}{T_M} \right) \quad (14)
\]

and \( Z_i/Z_a \) is the ratio of the electronic partition functions which can be approximated to be 6 for argon. The rate constants of argon \(^{12,13}\) used in the present numerical calculations are

\[
k_{ra}(T) = 5.80 \cdot 10^{-37} \cdot \frac{T_{A_1}}{T} + 2 \cdot \exp \left( - \frac{T_{ion} - T_{A_1}}{T} \right) \left( \frac{cm^6}{s} \right) \quad (15)
\]
where the characteristic temperatures of ionization and excitation are \( T_{\text{ion}} = 183100 \, ^\circ\text{K} \) and \( T_{\text{A1}} = 135300 \, ^\circ\text{K} \).

The elastic collision frequency between electrons and heavy particles \( v_{\text{eh}} \) is the sum of electron-ion collision frequency \( v_{\text{ei}} \) and electron-atom collision frequency \( v_{\text{ea}} \):

\[
v_{\text{eh}} = v_{\text{ei}} + v_{\text{ea}},
\]

\[
v_{\text{ei}} = \frac{e^2}{m_h} \left( \frac{8 k T_e}{m_e} \right)^{1/2} Q_{\text{ei}},
\]

\[
v_{\text{ea}} = \left( 1 - e^2 \right) \frac{e^2}{m_h} \left( \frac{8 k T_e}{m_e} \right)^{1/2} Q_{\text{ea}}.
\]

The elastic collision cross-section between electrons and atoms\(^{14}\) adopted in the present numerical calculations is

\[
Q_{\text{ea}} = \begin{cases} 
-0.35 + 0.775 \cdot 10^{-4} \cdot T_e \cdot 10^{-16}, & \text{cm}^2; \\
10^4 \, ^\circ\text{K} < T_e < 5 \cdot 10^5 \, ^\circ\text{K}; \\
(0.39 - 0.551 \cdot 10^{-4} \cdot T_e + 0.595 \cdot 10^{-8} \cdot T_e^2) \cdot 10^{-16}, & \text{cm}^2; \\
T_e < 10^4 \, ^\circ\text{K}
\end{cases}
\]

and the elastic collision cross-section for electrons and ions\(^{10}\) can be expressed as

\[
Q_{\text{ei}} = \frac{2 \pi e^4}{9 k^2 T_e^2} \ln \left( \frac{9 k^3 T_e^3}{4 \pi e^6 n_e} \right),
\]

### 2.3. Finite Difference Equations

As the aforementioned differential equations are of the form:

\[
\partial U/\partial t + \partial F(U)/\partial x = G,
\]

we can apply the two-step Lax-Wendroff scheme\(^{15}\) which is written as follows:

\[
U_j^{n+1} = U_j^n - \frac{\lambda}{2} \left[ \frac{1}{2} (F_j^{n+1} - F_j^n) + (F_j^{n+1}) \right] + G_{j+\frac{1}{2}}^{n+1} \Delta t,
\]

\[
G_{j+\frac{1}{2}}^{n+1} = G \left[ \frac{1}{2} (2 U_j^n + U_{j+1}^n + U_{j-1}^n) \right],
\]

\[
\tilde{F}_j^{n+1} = F (\tilde{U}_j^{n+1}),
\]

\[
\tilde{U}_j^{n+1} = \frac{1}{2} (U_j^{n+1} + U_{j+1}^n) - \frac{\lambda}{2} (F_j^{n+1} - F_j^n) + G_{j+\frac{1}{2}}^{n+1} \Delta t,
\]

\[
G_{j+\frac{1}{2}}^{n+1} = G \left[ \frac{1}{2} (U_{j+1}^{n+1} + U_j^n) \right]
\]

where the subscripts \( j \) and \( n \) refer to the grid points of \( x \)- and \( t \)-coordinates, \( \Delta x \) and \( \Delta t \) are the step sizes of them, and \( \lambda = \Delta t / \Delta x \) which must satisfy the Courant-Friedrich-Lewy condition\(^{16}\):

\[
\Delta t / \Delta x \leq 1 / \max(a + |u|)
\]

where \( a \) is the speed of sound given by

\[
a^2 = \frac{5}{3} \frac{p}{\rho}.
\]

### 2.4. Boundary Conditions and Initial Conditions

The wall is located at the grid point \( j = 0 \) corresponding to \( x = 0 \). As the condition of symmetry is hold at \( j = 0 \), \( U_j^n \) at the grid point \( j = -1 \) is determined in the following way:

\[
u_{-1}^n = -u_1^n, \quad v_{-1}^n = v_1^n, \quad p_{-1}^n = p_1^n,
\]

\[
e_{-1}^n = e_1^n, \quad e_{-1}^n = e_1^n.
\]

Then, \( U_j^{n+1} \) at \( j = 0 \) is evaluated from \( U_j^n \) at \( j = -1, 0 \) and 1 by Equation (23).

In order to shorten computation time, the computation domain is restricted within the zigzag area as shown in Figure 1. The conditions on the zigzag boundary are evaluated by the relation of \( U(x, t + \tilde{t}) = U(x + \tilde{U}, \tilde{t}) \).
Table 1. Conditions of numerical calculations: Incident shock Mach number, initial pressure, shock speed and step-sizes of finite difference scheme.

<table>
<thead>
<tr>
<th>Case</th>
<th>$M_s$</th>
<th>$p_i$</th>
<th>$U_s$</th>
<th>$\Delta x$</th>
<th>$\Delta t$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>16</td>
<td>1</td>
<td>5.16 km/s</td>
<td>0.1453 mm</td>
<td>0.01935 μs</td>
</tr>
<tr>
<td>2</td>
<td>14</td>
<td>3</td>
<td>4.52</td>
<td>0.1001</td>
<td>0.01519</td>
</tr>
<tr>
<td>3</td>
<td>12</td>
<td>5</td>
<td>3.87</td>
<td>0.1345</td>
<td>0.02372</td>
</tr>
</tbody>
</table>

![Fig. 2. Distance-time diagram of shock reflection processes for Case 1: $M_s = 16$ and $p_i = 1$ torr.](image2)

![Fig. 3. Distance-time diagram of shock reflection processes for Case 2: $M_s = 14$ and $p_i = 3$ torr.](image3)

![Fig. 4. Distance-time diagram of shock reflection processes for Case 3: $M_s = 12$ and $p_i = 5$ torr.](image4)

![Fig. 5. Nondimensional plots of the flow field behind the incident shock for Case 1, characteristic values are $x_0 = 2.91$ cm, $q_0 = 2.13 \times 10^{-6}$ g/cm³, $T_0 = 11913$ °K, $u_0 = 5.16$ km/s and $p_0 = 0.561$ atm.](image5)

Three cases are shown in Figures 2, 3 and 4. We shall explain the reflection processes mainly referring to Figure 2. Figure 5 shows the profiles of the incident-shock flowfield which consists of three main regions: the frozen region, the ionizing region and the equilibrium region. For a short time after the reflection of the incident shock, the shocked gas is in a frozen state. In the meantime, the ionization reaction proceeds in the frozen region and the reflected shock begins to move rather slowly. Then, the sudden onset of equilibration beginning at the end wall, the temperature falls down and the density increases in the equilibrium region adjacent to the end wall because the ionization reaction removes the ionization energy from the kinetic energy. Consequently,
expansion waves propagate away from the end wall and weaken the reflected shock. Figure 6 shows the computer plots of the reflected-shock flowfields at $t = 5.22 \mu s$: the reflected shock arrives at $x = 1.22 \text{ cm}$ ($\tilde{x} = 0.42$), the gas is in an equilibrium state near the end wall, $x = 0 \sim 0.15 \text{ cm}$ ($\tilde{x} = 0 \sim 0.05$), and the expansion wave has the minimum pressure at $x = 0.55 \text{ cm}$ ($\tilde{x} = 0.19$):

Figure 4 indicates that the reflected shock travels away from the end wall at the frozen speed immediately after reflection and subsequently it is decelerated to the equilibrium speed. This transient reflection process forms the nonuniform region near the end wall which is called as an entropy layer in vibrational or dissociative gases. The profiles of the electron number density of the reflected-shock flowfield are shown in Fig. 7 for several discrete times marked in Figure 4. The electron number density $n_{e\text{FE}}$ in Fig. 7 is calculated assuming the equilibrium reflected shock and the frozen incident shock. The electron number density adjacent to the wall exceeds the equilibrium value of $n_{e\text{FE}}$, because these gas particles are processed by a stronger frozen reflected shock than the equilibrium reflected shock. In the almost uniform region beyond the entropy layer ($x \gtrsim 1.1 \text{ cm}$), the number density of electrons attains slightly above the equilibrium value due to the influence of the ionization relaxation behind the incident shock.

As the gas in front of the reflected shock relaxes into equilibrium and its density increases, the reflected shock is decelerated and then, it goes back towards the end wall ($t = 15 \mu s$, in Figure 2). We shall discuss how the reflected shock propagating back to the end wall interacts with the equilibrium
Fig. 7. Profiles of the number density of electrons at discrete times after reflection:
(1) 1.07 µs, (2) 2.49 µs, (3) 5.34 µs, (4) 12.45 µs, (5) 19.57 µs, (6) 26.68 µs.

Fig. 8. Profiles of the pressure and the temperature of heavy particles for Case 2: Numbers 1, 2, 3 and 4 refer to 13.14 µs, 14.66 µs, 16.18 µs and 17.70 µs after reflection, respectively.

region behind it, referring to Figure 3. Typical profiles of the flowfield marked with 1, 2, 3 and 4 in Fig. 3 are shown in Figure 8. The reflected shock is denoted by 1R, 2R, etc. and the onset of equilibration is denoted by 1E, 2E, etc. The profile 1 shows the flowfield that the reflected shock almost ceases moving and the upstream gas is still in nonequilibrium. In the profile 2, the retiring shock weakening, the pressure and the temperature of the nonequilibrium region behind it are reduced. But the pressure in the neighborhood of 2E point grows high and the temperature of the relaxation region becomes higher at the last stage of relaxation because of the gas moving against the steep pressure gradient. In the profile 3, from the high-pressure zone (3E) between the equilibrium region and the nonequilibrium region, a compression wave (3C, 4C) is generated and propagates towards the end wall. Simultaneously a shock (3S) is also produced moving to the reflected shock. Colliding of this newly generated shock with the reflected shock gives rise to a contact surface where the density and the degree of ionization are discontinuous but the temperature is almost continuous.

The end-wall pressure history in Fig. 2 shows that there is an abrupt pressure increase at $t = $
17.8 μs. It is due to the reflection of the compression wave caused by the aforementioned interaction. Then, weak expansion waves are caused due to the secondary ionization relaxation ($t = 21.6 \mu s$) and follow after the reflected compression wave. The reflected compression wave catching up with the reflected shock strengthens it and propagates back as a weak expansion wave. At the same time, another contact surface is generated, where the density and the degree of ionization are again discontinuous but the temperature is almost continuous. The end-wall pressure decreases due to this expansion wave and then increases slightly to the equilibrium value of $p_{\text{eq}}$.

Figure 9 shows the computer plots of the hot stagnant region where the reflected shock passed through ($t = 36.18 \mu s$, in Figure 2). The pressure- and temperature-profiles are straightforward there, but the profiles of the density and of the degree of ionization are not so simple due to the interactions between ionization relaxation processes and waves.

3.2. Comparisons with Experiments and Discussions

Kuiper$^1,^5$ obtained the measurements of the time history of the electron number density and the mass density behind the reflected shock in ionizing argon by use of time-resolved Mach-Zehnder interferometry, and made the distance-time diagrams for the case of the initial pressure of $p_1 = 5$ torr and the incident shock Mach numbers of $M_s = 11.4$ and $M_s = 12.7$. The qualitative agreement with our distance-time diagram of Case 3 (Fig. 4) is good, while the quantitative comparison is inadequate because the relaxation times of the incident shocks in his experiments are shorter than those of our numerical results. Generally, in the experiments, the ionization relaxation time behind an incident shock is shortenned by several effects such as an impurity of test gases$^{17}$, an incident side-wall boundary layer$^{18}$ and so on. The ionization relaxation times in our calculations coincide with the experimental relaxation times by Wong and Bershader$^{19}$. It is also shown by Kuiper$^1$ that the measured electron number density at the edge of the boundary layer on the end wall is larger than the theoretical equilibrium one; for example, $n_e = 4.55 \cdot 10^{17} \text{ cm}^{-3}$ for the condition of $p_1 = 5$ torr and $M_s = 12$, and its equilibrium value is $n_{e\text{E}} = 3.98 \cdot 10^{17} \text{ cm}^{-3}$. Our results of Fig. 7 are comparable.

Smith$^3$ made the measurements of the pressure history in ionizing xenon with the fast-rise pressure gauge mounted in the end wall of the shock tube. The present results of the end-wall pressure history
shown in Fig. 2 gives a similar profile to his experimental one.

We have neglected the existence of Ar\(^{++}\)-ions in our numerical calculations. According to JPL Technical Report\(^{20}\), the concentration of Ar\(^{++}\)-ions behind the equilibrium reflected shock is less than 1 \(\times 10^{-3}\)\% in such a condition as in Table 1: for example, the number densities of Ar-atoms, Ar\(^{+}\) ions and Ar\(^{++}\)-ions behind the equilibrium reflected shock are 9.2 \(\times 10^{17}\) cm\(^{-3}\), 6.8 \(\times 10^{17}\) cm\(^{-3}\) and 2.5 \(\times 10^{13}\) cm\(^{-3}\) respectively, for the condition of the incident shock velocity \(U_s = 5.22\) Km/s, the initial pressure \(p_1 = 1\) torr and the initial temperature \(T_x = 300\) °K. Hence our dismissal of Ar\(^{++}\)-ions is valid.

In the present study, we have employed the formulas of ionization rates and collision cross-sections used by Hoffert and Lien\(^{11}\). It should be noted that the collision cross-section between electrons and atoms \(Q_{ea}\) discussed by Devoto\(^{21}\) is several times larger and the ionization rate due to atom-atom inelastic collisions \(k_{ia}\) determined by McLaren and Hobson\(^{22}\) is several factors smaller than those used here.

4. Conclusion

Numerical calculations of the ionizing shock reflection at a closed end of a shock tube have been performed by use of the two-step Lax-Wendroff scheme. Some interesting phenomena and complicated flowfields have been found out which occur due to the interaction between ionization relaxation processes and reflected shocks. The effects of radiation cooling and the interaction between a reflected shock and an incident side-wall boundary layer might have to be taken into consideration hereafter. The present finite difference procedure is applicable straightforward to solve the present problems including the radiation energy loss.