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SHOCK SLIP-RELATIONS FOR THERMAL AND CHEMICAL NONEQUILIBRIUM FLOWS*

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ABSTRACT: This paper appears to be the first where the multi-temperature shock slip-relations for the thermal and chemical nonequilibrium flows are derived. The derivation is based on analysis of the influences of thermal nonequilibrium and viscous effects on the mass, momentum and energy flux balance relations at the shock wave. When the relaxation times for all internal energy modes tend to zero, the multi-temperature shock slip-relations are converted into single-temperature ones for thermal equilibrium flows. The present results can be applied to flows over vehicles of different geometries with or without angles of attack. In addition, the present single-temperature shock slip-relations are compared with those in the literature, and some defects and limitations in the latter are clarified.

KEY WORDS: *shock slip, thermal nonequilibrium, multi-temperature*

1 INTRODUCTION

As a result of development of space flight and missile engineering the hypersonic reentry flows in the slip region become important research topics. Since the flows generally are of thermal and chemical nonequilibrium, the continuum treatment of the problems requires the employment of multi-temperature governing equations[1] and corresponding slip-boundary conditions. The author and Tao[2] first presented recently the multi-temperature wall slip-boundary equations for thermal and chemical nonequilibrium flows. The purpose of the present work is to derive the corresponding shock slip-boundary equations for these flows.

2 VARIOUS FLUX BALANCE EQUATIONS AT THE SHOCK

The analysis outlined herein contains the following assumptions:

(1) In the slip region it is still possible to treat the bow shock as a discontinuity surface, taking into account the viscous effects[3] (including viscosity, thermal conductivity

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and diffusion effects, similarly hereafter) behind the shock in the flux balance equations at the shock.

(2) When the free-stream velocity U_∞^* >8 km/s, the thermal radiation fluxes from the wall and gases of the shock layer may have influence on the state parameters of gases before the shock. It is assumed that the gas flows before the shock are in the thermal and chemical equilibrium. So hereafter the term "nonequilibrium" always relates to flows behind the shock. In addition the radiation fluxes across the shock are assumed constant.

(3) In the cases of thermal nonequilibrium flows the changes of fluxes of various internal energy modes (except translational mode for heavy particle species) in transit process of the flows across the shock are neglected.

(4) The translational temperatures of various heavy-particle species behind the shock are assumed equal to each other, and written as T_s.

(5) For the chemical nonequilibrium cases the chemical reactions of gas mixture in transit process of the flows across the shock are neglected.

In order to obtain simpler results we use the shock-fitted orthogonal coordinates $(\widetilde{x}^*, \widetilde{y}^*, \widetilde{z}^*)$ that at arbitrary point $\widetilde{A}(\widetilde{x}^*, \widetilde{z}^*)$ of the shock the directions of $\widetilde{y}^*$ and $\widetilde{x}^*$ are identical to those of the normal to the shock and projecting line of the U_∞^* on the tangent plane of the shock, respectively, while the direction of $\widetilde{z}^*$ is defined by left-hand rule. The corresponding velocity components are $(\widetilde{u}^*, \widetilde{v}^*, \widetilde{w}^*)$.

Employing the aforementioned assumptions, the general expressions of flux balance equations at $\widetilde{A}(\widetilde{x}^*, \widetilde{z}^*)$ for mass, normal momentum, tangential momenta, species mass, total energy and internal energies are derived from analysis of influences of the viscous effects and thermal nonequilibrium on the flux balance equations and written as follows:

$$\rho_s^* \widetilde{v}_s^* = -\rho_\infty^* U_\infty^* \sin\sigma \tag{1}$$

$$p_s^* + \rho_s^* (\widetilde{v}_s^*)^2 - \widetilde{\tau}_{\widetilde{yy}s}^* = p_\infty^* + \rho_\infty^* (U_\infty^*)^2 \sin^2\sigma \tag{2}$$

$$\widetilde{\tau}_{\widetilde{xy}s}^* - \rho_s^* \widetilde{v}_s^* \widetilde{u}_s^* = \rho_\infty^* (U_\infty^*)^2 \sin\sigma\cos\sigma \tag{3a}$$

$$\widetilde{\tau}_{\widetilde{zy}s}^* - \rho_s^* \widetilde{v}_s^* \widetilde{w}_s^* = 0 \tag{3b}$$

$$\widetilde{J}_{is}^* + \rho_s^* \widetilde{v}_s^* c_{is} = -\rho_\infty^* U_\infty^* c_{i\infty} \sin\sigma \qquad (i = 1 \sim NS, \text{ the same hereafter}) \tag{4}$$

$$\begin{aligned} &\widetilde{\rho}_s^* \widetilde{v}_s^* \{h_s^* + \frac{1}{2}[(\widetilde{u}_s^*)^2 + (\widetilde{v}_s^*)^2 + (\widetilde{w}_s^*)^2]\} + \widetilde{q}_s^* + \sum_i \widetilde{J}_{is}^* h_{is}^* - \\ &\qquad \widetilde{\tau}_{\widetilde{xy}s}^* \widetilde{u}_s^* - \widetilde{\tau}_{\widetilde{yy}s}^* \widetilde{v}_s^* - \widetilde{\tau}_{\widetilde{zy}s}^* \widetilde{w}_s^* = -\rho_\infty^* U_\infty^* \sin\sigma [h_\infty^* + \frac{1}{2}(U_\infty^*)^2] \end{aligned} \tag{5}$$

$$\left. \begin{aligned} &\rho_s^* \widetilde{v}_s^* c_{is} e_{kis}^* + \widetilde{q}_{kis}^* + \widetilde{J}_{is}^* e_{kis}^* + \dot{E}_{kis}^* = -\rho_\infty^* U_\infty^* c_{i\infty} e_{ki\infty}^* \sin\sigma \\ &k = \begin{cases} r, v, e & \text{for polyatomic species} \\ e & \text{for monoatomic species} \\ t & \text{for free-electron } e^- \end{cases} \end{aligned} \right\} \tag{6}$$

where σ is the angle between U_∞^* and $\widetilde{x}^*$; e_k^* the internal energy of mode k; $\dot{E}_{kis}^* \equiv \dot{E}_{kisf}^* -$

$\dot{E}^*_{kisb}$, and $\dot{E}^*_{kis}, \dot{E}^*_{kisf}, \dot{E}^*_{kisb}$ the net, forward, backward source rates per unit area for the mode k on account of energy exchange between the modes in transit process of the flows across the shock, and in the cases of thermal nonequilibrium we have $\dot{E}^*_{kis} = \dot{E}^*_{kisf} = \dot{E}^*_{kisb} = 0$ (see assumption (3)) while for the cases of thermal equilibrium we have $\dot{E}^*_{kisf}$ and $\dot{E}^*_{kisb}$, approaching to infinity (see par. 4); superscript $*$ — the 'dimensional'; subscript s — the 'post-shock'; subscript ∞ — the 'afore-shock' and it will be different from 'free stream' when the radiation fluxes mentioned in assumption (2) are remarkable; subscripts t, r, v, e and i — the translational, rotational, vibrational, electronic modes and species index respectively; affix $\sim$ — the 'shock-fitted coordinate system'. The other symbols are in common use and explanations for them are omitted.

3 NONDIMENSIONAL MULTI-TEMPERATURE SHOCK SLIP-RELATIONS

Equations (1) $\sim$ (6) with addition of the equation of state behind the shock are just the dimensional shock slip-relations in primary form. Employing the same nondimensionlization factors as in Ref.[4], the dimensionless multi-temperature shock slip-relations (MTSSR) are derived from the above dimensional equations as follows

$$\rho_s \widetilde{v}_s = -\sin\sigma \tag{7}$$

$$p_s - \widetilde{v}_s \sin\sigma - \widetilde{\tau}_{\widetilde{yy}s} = p_\infty + \sin^2\sigma \tag{8}$$

$$\widetilde{\tau}_{\widetilde{xy}s} + \widetilde{u}_s \sin\sigma = \sin\sigma\cos\sigma \tag{9a}$$

$$\widetilde{\tau}_{\widetilde{zy}s} + \widetilde{w}_s \sin\sigma = 0 \tag{9b}$$

$$\widetilde{J}_{is} - (c_{is} - c_{i\infty})\sin\sigma = 0 \qquad (i = 1\sim NS, \text{the same hereafter}) \tag{10}$$

$$\widetilde{q}_s - \sin\sigma\Big[\sum_i c_{i\infty}(h_{is} - h_{i\infty})\Big] + \frac{1}{2}\sin\sigma\Big[1 + \widetilde{u}_s^2 - \widetilde{v}_s^2 + \widetilde{w}_s^2 - 2\cos\sigma(\widetilde{u}_s + \widetilde{w}_s)\Big] - \widetilde{\tau}_{\widetilde{yy}s}\widetilde{v}_s = 0 \tag{11}$$

$$\widetilde{q}_{kis} - c_{i\infty}(e_{kis} - e_{ki\infty})\sin\sigma = 0 \qquad (k \text{ is that in (6)}) \tag{12}$$

$$\left.\begin{aligned} &p_s = \sum_i p_{is} = [\rho RT + \rho_{e^-} R_{e^-}(T_{te^-} - T)]_s \\ &R \equiv R_0^*/(\overline{M}^* C^*_{p\infty}) \qquad R_i \equiv R_0^*/(M_i^* C^*_{p\infty}) \end{aligned}\right\} \tag{13}$$

where

$$\widetilde{q}_s = \sum_i \sum_k \widetilde{q}_{kis} = -\varepsilon^2 \sum_i \sum_k K_{kis}\Big(\frac{\partial T_{ki}}{\partial \widetilde{y}}\Big)_s \qquad (k = t, r, v, e) \tag{14}$$

$$h_i = h_i^0 + R_i T_{ti} + \sum_k e_{ki} \qquad (k = t, r, v, e) \tag{15}$$

the expressions of thermal conductivity K_{ki} and internal energy e_{ki} are the same as those in Ref.[5], and we take $K_{ki} = e_{ki} = 0$ for such a species i, for which the K_{ki} and e_{ki} are meaningless, for example, $K_{ri} = e_{ri} = 0$ for atomic species i; the expressions for viscous stresses $\widetilde{\tau}_{\widetilde{x}\widetilde{y}s}, \widetilde{\tau}_{\widetilde{y}\widetilde{y}s}, \widetilde{\tau}_{\widetilde{z}\widetilde{y}s}$ and diffusion flux $\widetilde{J}_{is}$ must be consistent with those in the governing equations of the flows.

Equations (7)~(13) are the dimensionless MTSSR in general form, for which the number of unknown temperatures $NT = 1 + NS + 2NM$, where NM is the number of molecular species. The other simplified MTSSR can be derived easily from these relations. For the simplified cases that were mentioned in Ref.[2], Eqs.(7)~(11) remain the same, and Eqs.(12)~(15) can be simplified. For example, in case of five-temperature (translational, rotational, vibrational, electronic excitation and electron) model, assuming $T_{ki} = T_k(k = r, v, e)$ and combining all Eqs.(12) with identical T_k we reduce the number of Eqs.(12) from $(NS+2NM)$ to four, and rearranging all terms with the same T_k in Eqs.(14) and (15), we obtain the five-temperature shock slip-relations; in case of four-temperature (translational-rotational, vibrational, electronic excitation and electron) model, eliminating Eqs.(12) with $k = r$ and repeating the above simplification operations the four-temperature shock slip-relations are derived. Similarly, we can obtain the shock slip-relations for cases of three-temperature (translational-rotational, vibrational and electron-electronic excitation), two-temperature A (translational-rotational and vibrational-electron-electronic excitation) and two-temperature B (translational-rotational and vibrational) models.

For using the shock slip-relations to solve the governing equations, the coordinate transformation formulas for the above shock-fitted coordinate system and that used in the governing equations are required. In general 3-D cases these formulas can be found in Refs.[6,7].

When the flows are 2-D or axisymmetric, and the governing equations are viscous shock layer (VSL) ones of two-temperature A model, and when considering only the term concerning species mass fraction gradient for the diffusion fluxes and neglecting the terms with $\widetilde{\tau}_{\widetilde{y}\widetilde{y}}$, the above MTSSR can be simplified as:

$$\rho_s \widetilde{v}_s = -\sin\alpha \tag{16}$$

$$p_s - \widetilde{v}_s \sin\alpha = p_\infty + \sin^2\alpha \tag{17}$$

$$\varepsilon^2 \mu_s \Big(\frac{\partial \widetilde{u}}{\partial \widetilde{y}} - \widetilde{K}' \widetilde{u}\Big)_s + \widetilde{u}_s \sin\alpha = \sin\alpha \cos\alpha \tag{18}$$

$$\varepsilon^2 \rho_s D_{is} \Big(\frac{\partial c_i}{\partial \widetilde{y}}\Big)_s + (c_{is} - c_{i\infty}) \sin\alpha = 0 \tag{19}$$

$$\varepsilon^2 \Big(K_{\rm T} \frac{\partial T_{\rm T}}{\partial \widetilde{y}} + K_{\rm VE} \frac{\partial T_{\rm VE}}{\partial \widetilde{y}}\Big)_s + \sin\alpha \Big[\sum_i c_{i\infty}(h_{is} - h_{i\infty})\Big] - \frac{1}{2} \sin\alpha \Big[\big(\widetilde{u}_s - \cos\alpha\big)^2 + \sin^2\alpha - \widetilde{v}_s^2\Big] = 0 \tag{20}$$

$$\left.\begin{aligned} &\varepsilon^2 \Big(K_{\rm VE} \frac{\partial T_{\rm VE}}{\partial \widetilde{y}}\Big)_s + \sin\alpha \Big[\sum_i c_{i\infty} \sum_k (e_{kis} - e_{ki\infty})\Big] = 0 \\ &k = \begin{cases} v, e & \text{for polyatomic species} \\ e & \text{for monoatomic species} \\ t & \text{for free-electron } e^- \end{cases} \end{aligned}\right\} \tag{21}$$

$$p_s = [\rho R T_{\mathrm{T}} + \rho_{e^-} R_{e^-} (T_{\mathrm{VE}} - T_{\mathrm{T}})]_s \tag{22}$$

where α is the shock angle ($\sigma = \alpha$ for 2-D or axisymmetric flows); $\widetilde{K}'$ the shock curvature; D_i the effective diffussion coefficient of species i [5]; subscripts T and VE the translational-rotational and vibrational-electron-electronic excitation respectively; the other symbols are in common use for VSL equations[4] and explanations for them are omitted.

For 2-D or axisymmetric cases using the body-surface fitted orthogonal coordinates (x, y) in the governing equations, the transformation formulas for velocity components and partial derivatives in the two coordinate systems are as follows

$$\left.\begin{aligned}
\widetilde{u}_s &= u_s \cos(\alpha - \theta) + v_s \sin(\alpha - \theta) \\
\widetilde{v}_s &= -u_s \sin(\alpha - \theta) + v_s \cos(\alpha - \theta) \\
\left(\frac{\partial}{\partial \widetilde{x}}\right)_s &= \cos(\alpha - \theta)\left(\frac{\partial}{\partial x}\right)_s + \sin(\alpha - \theta)\left(\frac{\partial}{\partial y}\right)_s \\
\left(\frac{\partial}{\partial \widetilde{y}}\right)_s &= -\sin(\alpha - \theta)\left(\frac{\partial}{\partial x}\right)_s + \cos(\alpha - \theta)\left(\frac{\partial}{\partial y}\right)_s
\end{aligned}\right\} \tag{23}$$

where θ is body surface angle.

4 SHOCK SLIP-RELATIONS FOR THERMAL EQUILIBRIUM FLOWS AND COMPARISON WITH OTHER RESULTS

In the lower part of the slip region sometimes the gas flows in the shock-layer are thermal equilibrium and chemical nonequilibrium ones, so that consideration of the shock slip-relations for thermal equilibrium cases has practical interest. Moreover, the obtained results can be used for comparison with those in literature.

When all the relaxation times of internal energy modes are much less than the transit time of the flows (or we say that the former tends to zero), the state of the gas flows is converted from thermal nonequilibrium to thermal equilibrium in a very thin layer behind the shock, while the chemical reactions are still negligible (since the number of particle collisions are not high enough to produce noticeable reactions) in transit process of the flows across the layer. Because the thickness of this layer can be neglected, it is reasonable to consider the layer together with the shock, so that we have an 'effective shock', for which the thermal nonequilibrium shock slip-relations must be replaced by the thermal equilibrium ones.

On the basis of the above analysis the shock slip-relations for thermal equilibrium cases can be derived easily from the general flux balance Eqs.(1)~(6) and state Eq.(13). In these cases the orders of magnitude of $\dot{E}^*_{kisf}$ and $\dot{E}^*_{kisb}$ are much greater than those of all other terms (or we say that $\dot{E}^*_{kisf}$ and $\dot{E}^*_{kisb}$ approach to infinity) in Eqs.(6), so that Eqs.(6) are converted into identicals, which must be replaced by the following thermal equilibrium relations

$$T_{kis} = T_s \qquad (i = 1 \sim NS \qquad k \text{ is the same as that in Eqs.(6)}) \tag{24}$$

Substituting Eq.(24) into Eqs.(1)~(5) and (13), we obtain the general dimensionless single-temperature shock slip-relations (STSSR), in which the mass, normal momentum, tangential momenta and species mass flux balance equations are the same as Eqs.(7)~(10) respectively, while the energy flux balance and state equations are as follows

$$\varepsilon^2\Big(K\frac{\partial T}{\partial \widetilde{y}}\Big)_s + \sin\sigma\Big[\sum_i c_{i\infty}(h_{is} - h_{i\infty})\Big] - \frac{1}{2}\sin\sigma[1 + \widetilde{u}_s^2 - \widetilde{v}_s^2 + \widetilde{w}_s^2 - 2\cos\sigma(\widetilde{u}_s + \widetilde{w}_s)] - \widetilde{\tau}_{\widetilde{y}\widetilde{y}}\widetilde{v}_s = 0 \tag{25}$$

$$p_s = (\rho RT)_s \tag{26}$$

For the axisymmetric or 2-D cases, which are similar to those for two-temperature A model in par. 3, from the above STSSR we obtain the simplified relations, in which the mass, normal momentum, tangential momenta, species mass flux balance and state equations are identical to Eqs.(16)~(19) and (26) respectively, while the energy flux equation is simplified as

$$\varepsilon^2\Big(K\frac{\partial T}{\partial \widetilde{y}}\Big)_s + \sin\alpha\Big[\sum_i c_{i\infty}(h_{is} - h_{i\infty})\Big] - \frac{1}{2}\sin\alpha\Big[(\widetilde{u}_s - \cos\alpha)^2 + \sin^2\alpha - \widetilde{v}_s^2\Big] = 0 \tag{27}$$

Comparing the single-temperature shock slip-relations of this paper with those in Refs.[4,8~11], the following main points deserve notice:

(1) In the shock slip-relations of the above literatures the differences of velocity components in the shock-fitted and body-surface fitted coordinate systems are accounted for, but the differences of partial derivatives of velocity components, temperatures, species mass fractions with respect to spatial coordinates in the above two coordinate systems are not considered. It can be seen from Eqs.(23) that the latter differences are magnitudes of the same order as the former, so that neglect of the latter differences is unreasonable, and it can result in remarkable errors in the shock slip-relations when the directions of corresponding coordinates of the two coordinate systems are very different (e.g., in the leeward side of the 3-D flows with large angles of attack).

(2) In the expressions of shear-stress components the terms concerning shock curvatures (the $\widetilde{K}_s'\widetilde{u}_s$ of Eq.(18) for axisymmetric or 2-D flows) are omitted in the shock slip-relations of the above literature. It is unreasonable due to the following facts: the above shock curvature terms generally have the same order of magnitude as the corresponding terms (the $K'u/(1+K'y)$ for axisymmetric or 2-D flows) in the governing equations, and the latter terms are always accounted for; in addition, the results of numerical solutions[4,9] show that the normal gradient of tangential velocity decreases rapidly from the wall to the shock, so that in the vicinity of the shock sometimes $\dfrac{\partial u}{\partial y} < K'u/(1+K'y)$ are possible.

(3) In comparison with the shock slip-relations of Refs.[10,11], the Eq.(9b) and the terms containing $\widetilde{w}_s$ in Eq.(25) are new. They must be considered in view of the following fact: For flows over vehicles of complex geometries with large angles of attack, sometimes it is possible that the post-shock stream lines and the corresponding afore-shock ones have no coplanarity, so that $\widetilde{w}_s \neq 0$. In addition, for general 3-D cases we take into account also the terms with $\widetilde{\tau}_{\widetilde{y}\widetilde{y}}$, which are neglected in the above literature.

5 CONCLUSIONS

(1) The MTSSR are first derived in this paper from analysis of the influences of thermal nonequilibrium and viscous effects on the mass, momentum and energy flux balance relations at the bow shock wave, and the simplifications of them for some practical cases are discussed.

(2) The general expressions of the shock slip-relations presented here are applicable for solving the governing equations of several types (NS, PNS and VSL) with shock-fitting algorithm, and for flows over vehicles of complex geometries with or without angles of attack.

(3) The shock slip-relations presented here are free from the coordinate system adopted in the governing equations, and the latter influences only upon the complemental formulas for transformation of velocity components and partial derivatives in different coordinate systems.

(4) When the relaxation times for all internal energy modes approach to zero, the MTSSR are converted into the STSSR, which are compared with those in the literature and some defects and limitations in the latter are indicated.

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