BLUNT BODY IN SUPERSONIC FLOW OF GAS MIXTURE WITH CHEMICAL REACTIONS

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An analysis is conducted of the case of a blunt axially symmetric body in a stationary flow of gas mixture with equilibrium chemical conditions for $M_\infty > 1$. In the solution the method of integral relations [1] is employed.

1. In the curvilinear coordinate system s, n, where s is the arc length of the body and n is the distance along the normal to the body (Fig. 1) the following equations govern the motion of an inviscous, thermally nonconductive gas:

$$\frac{\partial}{\partial s}(r\rho v)+\frac{\partial}{\partial n}(Ar\rho u)=0; \tag{1.1}$$

$$v\frac{\partial v}{\partial s}+Au\frac{\partial v}{\partial n}+Kuv+\frac{1}{\rho}\cdot\frac{\partial p}{\partial s}=0; \tag{1.2}$$

$$v\frac{\partial u}{\partial s}+Au\frac{\partial u}{\partial n}-Kv^2+\frac{A}{\rho}\cdot\frac{\partial p}{\partial n}=0. \tag{1.3}$$

The above can be brought to divergence form [1]:

$$\frac{\partial}{\partial s}(\bar{t})+\frac{\partial}{\partial n}(A\bar{l})=0; \tag{1.4}$$

$$\frac{\partial}{\partial s}(\bar{g})+\frac{\partial}{\partial n}(A\bar{z})=\bar{X}; \tag{1.5}$$

$$\frac{\partial}{\partial s}(\bar{z})+\frac{\partial}{\partial n}(A\bar{L})=\bar{Y}. \tag{1.6}$$

The following notation has been introduced in the above [1]:

$$\bar{z}=rz=r\rho uv;\ \bar{t}=rt=r\rho v;\ \bar{l}=rl=r\rho u;\ \bar{L}=rL=r(p+ru^2);$$
$$Y=K\bar{g}+A\cos\theta;\ \bar{g}=r(p+\rho v^2);\ A=1+Kn;\ r=r_0+n\cos\theta;$$
$$\bar{X}=-K\bar{z}+Ap\sin\theta.$$

The equations have been written in dimensionless form. The units of the variables ω, ρ, p, T, h, S, μ, s, n have been taken to be, respectively: ω_{max}, ρ_∞, $\rho_\infty v^2_{max}$, $\omega_{max}\mu_\infty/R$, $\omega^2_{max}/2$, $R/2\mu_\infty$, μ_∞, R_0.

Additional equations:

$$h+\omega^2=1; \tag{1.7}$$

$$Tds=dh-2\frac{dp}{\rho}; \tag{1.8}$$

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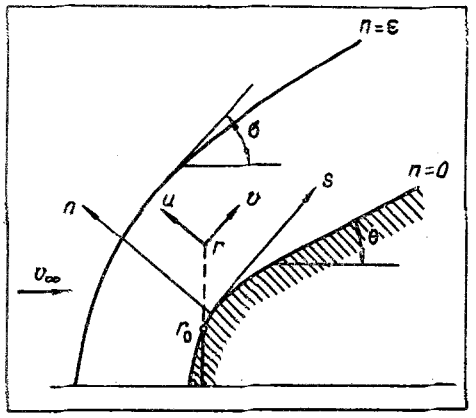

Fig. 1. A body-fixed coordinate system.

$$h=h(p,\ T); \tag{1.9}$$

$$\rho=\rho(p,\ T). \tag{1.10}$$

The system (1.4)-(1.10) is solved by using the method of integral relations [1]. One draws N – 1 intermediate curves between the body and the wave:

$$n_i=\varepsilon(s)\,\frac{N-i+1}{N};\ i=2,\ \ldots,\ N;\ n_0=0;\ n_1=\varepsilon(s). \tag{1.11}$$

The functions $\bar{z}$, $\bar{t}$, $\bar{g}$, $\bar{L}$, $\bar{Y}$, $\bar{l}$, $\bar{X}$ are now approximated by polynomials of degree N in the variable n. The substitution of the polynomials in Eqs. (1.4)-(1.6) and subsequent integration of the equations with respect to n from n = 0 to $n = n_i$ produces a system of ordinary differential equations for the unknown functions along each strip $n = n_i(s)$. If these equations are solved for v', u', p', T', ρ' one obtains equations for the unknown parameters. Below certain equations which will prove useful later on are given; the complete system can be found in [1].

N = 1 (the first approximation):

$$\begin{gathered}
\bar{t}_0'=\frac{\varepsilon'}{\varepsilon}(\bar{t}_1-\bar{t}_0)-\frac{2}{\varepsilon}(A_1\bar{l}_1-\bar{l}_0)-\bar{t}_1';\\
\bar{z}_1'=\frac{\varepsilon'}{\varepsilon}\bar{z}_1-\frac{2}{\varepsilon}(A_1\bar{L}_1-A_0\bar{L}_0)+(Y_0+Y_1);\\
N=1,\ 2;\ v_0'=E_0/N_0;\ v_2'=E_2/N_2;\\
E_0=\frac{1}{r_0}(\bar{t}_0'-r_0'\bar{t}_0);\\
E_2=\frac{1}{r_2}(\bar{t}_2'-r_2'\bar{t}_2)+\frac{\bar{z}_2'-\bar{t}_2'u_2}{r_2c_2^2}u_2-\left(\frac{vDB}{h_T}\right)_2;\\
u_2'=\frac{1}{\bar{t}_2}(\bar{z}_2'-\bar{t}_2'u_2);\\
B=\left(\frac{\partial p}{\partial n}+\rho\left(u\frac{\partial u}{\partial n}+v\frac{\partial v}{\partial n}\right)\right)\left(\frac{\varepsilon'}{2}-A_2\frac{u_2}{v_2}\right).
\end{gathered} \tag{1.12}$$

The system (1.12) is an approximation of (1.4), (1.6)-(1.9). Equation (1.8) was taken on the current curve and was projected on the curves $n = n_i$.

2. The conditions on the body, on the intersection of the shock wave and the symmetry axis, and on the symmetry axis are formulated in the usual way. Along the shock wave these conditions can be written as

$$\begin{gathered}
\frac{d\omega_n}{d\sigma}=\frac{\omega_\infty h_T\cos\sigma-\omega_n(D_1\Phi+\rho_T\Phi_1)}{\rho h_T-\omega_n(D_1\omega_\infty\sin\sigma-2\rho_T\omega_n)};\\
\frac{dp}{d\sigma}=\Phi-\omega_\infty\sin\sigma\,\frac{d\omega_n}{d\sigma};\\
\frac{dS}{d\sigma}=-\frac{2}{T}\left[\omega_n\frac{d\omega_n}{d\sigma}+\frac{1}{\rho}\cdot\frac{dp}{d\sigma}-\frac{\Phi_1}{2}\right];\\
D_1=(\rho_p h_T-\rho_T h_p);\ n=\varepsilon(s);\\
\Phi_1=\omega_\infty^2\sin 2\sigma;\ \Phi=\Phi_1-\omega_n\omega_\infty\cos\sigma,
\end{gathered} \tag{2.1}$$

where ω_i, ω_n are tangential and normal to the shock wave velocity components; σ, θ are angles between the shock wave and body contour, respectively, and the symmetry axis; h_T, h_p, ρ_T, ρ_p are partial derivatives of h, ρ with respect to T and p. The following conditions hold on the singular curve (v = c):

$$E_0=0, \quad \text{if} \quad N_0=0; \; E_2=0, \quad \text{if} \quad N_2=0. \tag{2.2}$$

The approximating system is now solved in the following order. The values $\varepsilon(0)$, $u_2(0)$ are given. The parameters $p_0(0)$, $T_0(0)$, $p_2(0)$, $T_2(0)$ are found using the system (2.3) which determines the distribution of parameters on the symmetry axis:

$$\frac{dp}{dn} = -\rho u \frac{du}{dn}; \qquad \frac{dT}{dn} = -\frac{1}{h_T}(\rho h_T - 2) u \frac{du}{dn}. \tag{2.3}$$

Subsequently, the system (1.12) and (2.1) can be integrated.

3. The point s = 0 is singular for some solutions of the system (1.12). Close to s = 0 the solution is sought in the form

$$f(s, n) = \sum_{k=1}^{m} f_k(0, n) s^k + 0(s^m). \tag{3.1}$$

If (3.1) is inserted in Eqs. (1.1)-(1.3) and (1.7)-(1.10), then, taking terms up to $0(s^3)$, we obtain the system:

$$\begin{gathered} v_1^2\rho_0 + Au_0\rho_0 \frac{\partial v_1}{\partial n} + \rho_0 K u_0 v_1 + 2p_2 = 0; \\ 2v_1u_2\rho_0 + Au_0\rho_2 \frac{\partial u_0}{\partial n} + Au_0\rho_0 \frac{\partial u_2}{\partial n} + Au_2\rho_0 \frac{\partial u_0}{\partial n} - Kv_1^2 + A \frac{\partial p_2}{\partial n} = 0; \\ \rho_2 T_0 + \rho_0 T_2 = p_2\mu_0 + p_0\mu_2; \\ h_p p_2 + h_T T_2 + 2u_0u_2 + (v_1)^2 = 0; \\ \mu_2 = \Sigma\mu_i \left[T_2 \frac{\partial x_i}{\partial T} + p_2 \frac{\partial x_i}{\partial p} \right]. \end{gathered} \tag{3.2}$$

The expansion coefficients in (3.1) are the unknowns in Eqs. (3.2). If, as previously, $f_k(n)$ is approximated by polynomials in n, there results a system for determining f_k which can be solved together with the system (1.12). By using (3.1) a solution can be obtained close to s = 0; it can subsequently be continued by integrating the basic system (1.12). For frozen chemical reactions $h_p = x_T = x_p = 0$ and the system (3.2) becomes less involved.

4. To solve the problem it is necessary to find the values $\varepsilon(0)$ and $u_2(0)$ for N = 2 or $\varepsilon(0)$ for N = 1 such that, as the result of the integration of the system (1.12) on the singular line, the condition (2.2) is satisfied. Suppose that, at the iteration k, we have $\varepsilon^{(k)}(0)$, $u_2^{(k)}(0)$. Then using them as the initial data, we may begin to integrate the system (1.12). The following alternatives may occur when approaching the singular line. At the point $s_i = s_{i1}$ (i = 0, 2)

$$E_i(s_{i1}) \leqslant \delta; \; N_i(s_{i1}) > \delta; \tag{4.1}$$

$$E_i(s_{i1}) \geqslant N_i(s_{i1}); \; N_i(s_{i1}) > \delta; \tag{4.2}$$

$$E_i(s_{i1}) \leqslant \delta; \; N_i(s_{i1}) \leqslant \delta. \tag{4.3}$$

In the case of (4.1)-(4.2) we are far away from the singular point and the solution cannot be continued for $s > s_i$ since it would not make sense from the physical point of view $|v_i'| = |E_i/N_i| \to \infty$. Close to singular points $v_i = c_i$ the condition (4.3) is satisfied. In this case the numerical error increases during the process of finding v_i' since $N_i \to 0$. Therefore we proceed in the following manner. The values $E_i(s - m\Delta s)$, $N_i(s - m\Delta s)$ serve to construct the polynomials

$$N_i = \sum_m N_{im} s^m; \tag{4.4}$$

$$E_i = \sum_m E_{im} s^m. \tag{4.5}$$

Extrapolating the singular points s_i are found from Eq. (4.6):

$$N_i(s)=0,\ i=0,\ 2 \tag{4.6}$$

and $E_i(s)$ from (4.5); subsequently, we proceed exactly as in the cases (4.1)-(4.2). By variation of the parameters $\varepsilon(0)$, $u_2(0)$ the relations (2.2) will be satisfied.

To cross a singular point at which $E_i = N_i = 0$ one can integrate the system obtained from (1.12). If the indeterminacy in the equation is eliminated by

$$v_0' = E_0/N_0 \quad \text{for} \quad E_0 \to 0,\ N_0 \to 0,\ v_0 \to c_0$$

and if to this is added the equations obtained by differentiation of the main system, then for $v_0 \to c_0$ the following system of equations results:

$$\begin{gathered}
v_0' - \frac{\rho'' v + \rho v'' + 2\rho' v'}{\frac{2\rho}{c}(c'-v')} = 0; \\
\rho'' + \rho v v'' = 0;\ \mu p - \rho R T = 0; \\
h_{pp}(p')^2 + h_p p'' + h_{TT}(T')^2 + h_T T'' + 2(v')^2 + 2vv'' = 0; \\
\frac{p''}{p} - \frac{\rho''}{\rho} - \frac{T''}{T} + \frac{\mu''}{\mu} - \left(\frac{p'}{p}\right)^2 + \left(\frac{\rho'}{\rho}\right)^2 + \left(\frac{T'}{T}\right)^2 - \left(\frac{\mu'}{\mu}\right)^2 = 0; \\
\frac{p'}{p} - \frac{\rho'}{\rho} - \frac{T'}{T} + \frac{\mu'}{\mu} = 0;\ p' + \rho v v' = 0; \\
p' - \rho' c^2 = 0;\ p'' - \rho'' c^2 = 2cc'\rho';\ h_p p' + h_T T' + 2vv' = 0.
\end{gathered} \tag{4.7}$$

From this system v_0'', p_0'', ρ_0'', v_0', p_0', ρ_0' and other values close to $v_0 = c_0$ can be determined. Similar formulas can be obtained for v_2.

5. Computation of the Parameters of the Mixture Dependent on Chemical Reactions. To be able to calculate $h(p, T)$, $\rho(p, T)$, $\mu(p, T)$, h_p, h_T, ρ_p, ρ_T it is necessary to know the mixture composition and also the total of chemical reactions taking place in the gas. In the case of equilibrium chemical reactions then for a specific fixed set of components, there may be different equivalent sets of independent chemical reactions. In our case the gas composition was as follows: $x_1 = CO_2$, $x_2 = CO$, $x_3 = H_2O$, $x_4 = H_3$, $x_5 = O_2$, $x_6 = OH$, $x_7 = O$, $x_8 = H$ (x_i are the component molar concentrations, n_{i1}, n_{i2}, n_{i3} are the number of O, C, H atoms in the component x_i). The set of independent chemical reactions is now fixed as follows:

$$\begin{gathered}
H_2 \rightleftarrows 2H - 103264 \text{ kcal/kmole}; \\
O_2 \rightleftarrows 2O - 117973; \\
O + H_2 \rightleftarrows OH + H - 1904; \\
OH + H_2 \rightleftarrows H_2O + H + 14737; \\
CO + O \rightleftarrows CO_2 + 125753.
\end{gathered} \tag{5.1}$$

Then for determining x_i the system of equations will consist of the Dalton equation (5.2), the equations expressing the conservation of the number of atoms (5.3)-(5.4) and the law of active masses (5.5)-(5.9):

$$\Sigma x_i = 1; \tag{5.2}$$

$$\frac{\Sigma n_{i2} x_i}{\Sigma n_{i1} x_i} = \frac{\Sigma n_{i2} x_{i\infty}}{\Sigma n_{i1} x_{i\infty}}; \tag{5.3}$$

$$\frac{\Sigma n_{i3} x_i}{\Sigma n_{i1} x_i} = \frac{\Sigma n_{i3} x_{i\infty}}{\Sigma n_{i1} x_{i\infty}}; \tag{5.4}$$

$$x_4 = F_4 \frac{x_2 x_3}{x_1}; \tag{5.5}$$

$$x_5 = F_5 \frac{x_1^2}{x_2^2 p}; \tag{5.6}$$

$$x_6 = F_6 \sqrt{\frac{x_1 x_3}{x_2 p}}; \tag{5.7}$$

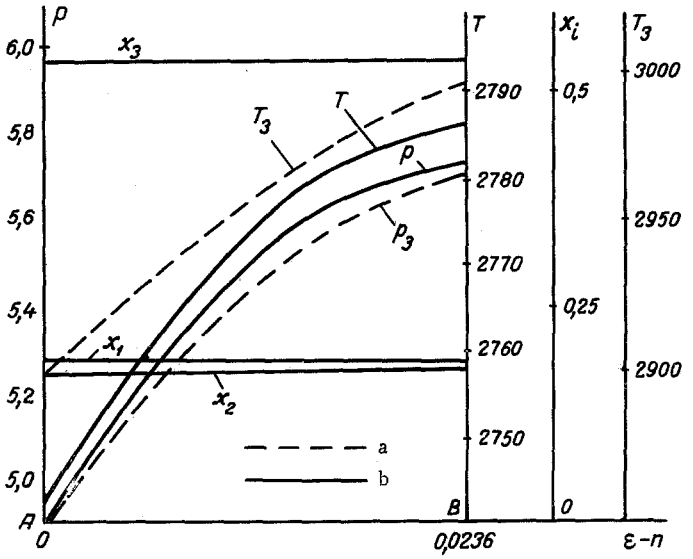

Fig. 2. Distribution of parameters on the symmetry axis between the shock wave A and the body B. T, °K; p, atm; a) frozen reactions; b) equilibrium reactions.

$$x_7 = F_7 \frac{x_1}{x_2 p}; \tag{5.8}$$

$$x_8 = F_8 \sqrt{\frac{x_2 x_3}{x_1 p}}. \tag{5.9}$$

The equations of the law of active masses are solved for the components x_4-x_8. In the above $F_i = F_i(K_{pi})$, where K_{pi} are the equilibrium constants of the reaction (5.1).

The system (5.2)-(5.9) is now solved in the following manner. For some fixed values of p and T we select m predominating components where m is the number of elements in the mixture. Let the predominating components be x_1, x_2, x_3. Equations (5.2)-(5.4) are now written in the form

$$\sum_{j=1}^{3} a_{ij} x_j = \sum_{j=4}^{8} a_{ij} x_j, \quad i = 1, 2, 3. \tag{5.10}$$

The nonlinear system (5.2)-(5.9) is solved by Newton's method. Taking $x_j = 0$, $j = 4, \ldots, 8$ as the initial approximation, x_j is calculated, for $j = 1, 2, 3$, using (5.10). Having found all x_i the remaining mixture parameters are now determined:

$$h = \frac{1}{\mu} \Sigma H_i(T) x_i;$$

$$\mu = \Sigma \mu_i x_i;$$

$$h_p = \frac{1}{\mu} \left(\Sigma H_i x_{ip} - \frac{H}{\mu} \Sigma \mu_i x_{ip} \right);$$

$$h_T = \frac{1}{\mu} \left(\Sigma x_i \frac{\partial H}{\partial T} + \Sigma H_i x_{iT} - \frac{H}{\mu} \Sigma \mu_i x_{iT} \right); \tag{5.11}$$

$$\rho_p = \frac{1}{T} (\mu + p \Sigma \mu_i x_{ip});$$

$$\rho_T = \frac{p}{T} \left(\Sigma \mu_i x_{iT} - \frac{\mu}{T} \right);$$

$$H_i(T) = [H_i(T) - H_i(0)] + \Delta H_i^0(0).$$

The quantities x_{ip}, x_{iT} in (5.11) are determined from the system (5.2)-(5.9), after differentiating with respect to p and T; $H_i(T)$ are molar enthalpies of the components; ΔH_i^0 is the enthalpy of the formation of component i, extrapolated to 0°K. The values of ΔH_i^0 are shown in Table 1.

TABLE 1. Values of ΔH_i^0, kcal/mole

x_i	CO_2	CO	H_2O	H_2	O_2	OH	O	H
ΔH_i^0	0	0	0	—9656	133533	71197	125753	46804

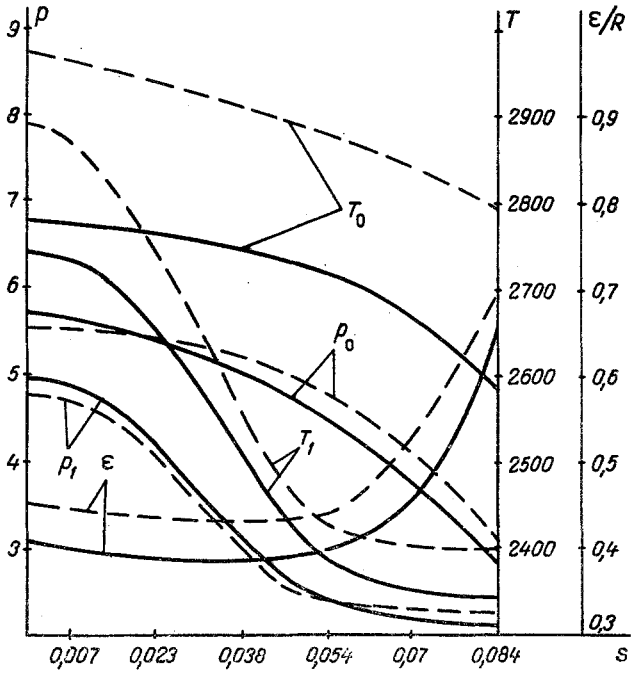

Fig. 3. Parameter distribution along the body and along the shock wave p, atm; T, °K.

The values of K_{pi}, H_i have been calculated using the approximations given in [5].

6. The method presented in Sections 1-5 is used to solve the following problem. A sphere together with a cone (its semivertical angle being 9°) flows in an equilibrium gas mixture with $v_\infty = 2010$ m/sec, $T_\infty = 2060°K$, $p_\infty = 1$ atm, $M_\infty = 2.14$, $R_0 = 0.06$ m. The calculation was performed in the first approximation (N = 1). Figures 2 and 3 show the distribution of pressure, temperature, and concentration of the main components on the symmetry axis along the body and along the shock wave.

The error in the calculations (N = 1) of the mixture parameters was about 10%. Since the parameters were approximated linearly on the midline, close to the singular points the flow map differs from the correct one in the values of v_2 and the position of the Mach line. The solution of the problem (N = 1) when not even an approximate value of $\varepsilon(0)$ is known, takes several hours on a Minsk-22 computer. The time required for one iteration is 20 min. The calculation of the mixture composition takes up to 80% of the total calculation time. Therefore the mixture composition and the thermodynamic parameters should be calculated in advance for a whole range of values of p and T and the tables or approximations thus produced used in the main calculations.

NOTATION

s, n are coordinates tangential and normal to the generating line of the body;
v, u are velocity components in the direction of s, n axes, m/sec;
r, r_0 are the distances between a point in the flow or a point in the body and the symmetry axis, m;
K, R are the dimensionless curvature and radius of curvature of a body contour;
ρ is the density, kg/m^3;
p is the pressure, atm;
T is the temperature, °K;
h is the total enthalpy of the mixture, kcal/kg;
μ is the molecular weight of the mixture;
S is the entropy of the mixture, kcal/kg · deg K;

c is the velocity of sound, m/sec;
ε is the removal of the shock wave, m;
x_i are the molar concentrations of the components.

Subscripts

0 denotes the body;
1 denotes the shock wave;
2 denotes the midline between body and wave;
' denotes differentiation with respect to the coordinate s.

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