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INVESTIGATION TO DEFINE THE PROPAGATION CHARACTERISTICS OF A FINITE AMPLITUDE ACOUSTIC PRESSURE WAVE

PHASE 1
FINAL REPORT

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FOREWORD

This report presents work performed by North American Aviation, Inc., Space and Information Systems Division, for the National Aeronautics and Space Administration Marshall Space Flight Center, Huntsville, Alabama, in fulfillment of Contract NAS8-11441, "An Investigation to Define the Propagation Characteristics of a Finite Amplitude Acoustic Pressure Wave."

Dr. Francis C. Hung acted as Program Manager for North American Aviation, Inc. Dr. T. C. Li and Mr. A. C. Peter were the investigators on the project.

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TECHNICAL REPORT INDEX/ABSTRACT

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AN INVESTIGATION TO DEFINE THE PROPAGATION CHARACTERISTICS OF A FINITE AMPLITUDE PRESSURE WAVE	

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ABSTRACT

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The contribution of high entropy production regions to the generation and propagation characteristics of a finite amplitude pressure wave is considered. Preliminary analysis indicates that, for nozzles where pressure ratios are above critical, the predominant contribution may come from the shock layer formation in the exhaust region. Temperature effects indicate high dependence of the forcing function upon the initial temperature of the media.

Author

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INTRODUCTION

The preliminary phase of the investigation of the propagation characteristics of a finite amplitude pressure wave, as pertaining to the conditions existing in the exhaust of a rocket nozzle, has been concerned with qualitative and, to some extent, quantitative analysis of the predominant dissipation terms. These dissipation terms, as evidenced by recent developments, may contribute heavily to the nonlinear wave radiation of rocket exhausts.

In this phase of the investigation, emphasis was placed on pinpointing, by means of general qualitative analysis, those regions of rocket exhausts in which the rate of entropy production is maximized. Thus, the present formulation is directed toward the analysis of those regions in which the physical processes are highly irreversible, with a consequent strong coupling between the mechanical and thermodynamic phenomena. It follows that those processes in which no entropy production occurs are automatically excluded from our consideration.

In terms of the mathematical formulation, the aforementioned approach implies a strong coupling between the momentum equation (mechanical conditions) and energy equation (thermodynamic conditions). The derivation of the governing equations in Section I of this report results in a wave equation (mechanical conditions) whose forcing function, in terms of entropy gradients, depends primarily upon dissipation processes; i.e., entropy production rates. As a consequence, the present approach tends to supplement the contemporary investigations on the subject.[1]

The preceding formulation points to the fact that, subject to future experimentation and within the framework of this analysis, the presence of Mach discs in a rocket exhaust nozzle may constitute the predominant acoustic propagation regions of the flow field, due to the high rates of entropy production there. This is true irrespective of cold or hot flow conditions—the temperature difference having the effect of magnifying the phenomena.

Other regions in which dissipation rates are predominant, even though not quite of the same order of magnitude as those in the Mach-disc transition regions, are the oblique shock layers formed in the rocket exhaust flow field. To analyze these regions for the case of high pressure-ratio rocket exhaust, recent hypersonic continuum mechanics developments have been employed and are presented in Section II of this report. An analysis of power-law oblique

[1] Refer to References and Bibliography.

shocks for small angle of inclinations tends to predict that the entropy close to the axis of symmetry increases rapidly, whereas the pressure remains quite uniform there. Because of the much higher entropy in layers near the axis, the temperature must be high and the density low. In this formulation, the transition properties are used as boundary values for the similarity solution of the wave equation.

In Section III of this report, the reflection properties of the pressure waves emanating from a rocket exhaust have been studied through use of characteristics in the physical and hodograph planes, with a view toward finding the point of coalescence of the pressure waves, which are reflected from the free boundary. These numerical computations result in a theoretical prediction of the shock wave shapes emanating from the rocket nozzle.

Regions in which entropy generation takes place through vortex interaction seem, within the framework of this analysis, to be of lesser importance in supersonic flow. They only become primary factors in acoustic excitation in subsonic flow, when no localized high-entropy production regions (i.e., shock fronts) exist.

The formal derivation of the forcing function, in terms of the dissipation processes presented in Section I, is based upon the assumption of the existence and continuity of the functions up to and including second derivatives as well as nondeviation from thermodynamic equilibria of the medium. In reality, the regions of high entropy-production rates are very often distinguished by their departure from thermodynamic equilibrium, especially in highly supersonic rocket exhausts and in the presence of nearly normal shock layers; i.e., Mach discs. Under these conditions, the conventional entropy definition based upon nondeviation from thermodynamic equilibrium usually is not sufficient. In such cases, the entropy function must take into account the energy states of the individual particles (i.e., atoms and molecules) since the rate of relaxation time to achieve local equilibrium varies, depending upon the molecular and atomic structures and the processes involved. In regions of high excitations, thermodynamic equilibrium may not be fully established because relaxation time may be considerably longer than the reciprocal of the mean of the collision frequency of the gas particle for the translational degree of freedom. Under such conditions of chemical flow processes, the entropy function has to be treated by statistical methods.

On the other hand, even when the chemical equilibrium is very nearly attained (i.e., when the rate of dissociation of molecules into atoms can be assumed to be equal to the rate of production of new molecules by recombination), there is a marked difference in the irreversibility of the process when transmission through a shock wave occurs. In Section IV of this report, a quantitative analysis of such transmission phenomena for binary collisions is presented for two different values of the mass fraction parameter. For comparison purposes, the transition values of entropy production for frozen flow (i. e., chemically inert flow) also have been included. It is seen that entropy production is considerably higher when dissociation and recombination take place, even under the conditions of chemical equilibrium. In addition, the entropy production rate is a strong function of the mass fraction; i. e., of the ratio by weight of atoms dissociated to the total weight of atoms and molecules. However, since this mass fraction depends explicitly upon the gas temperature, it follows that entropy production in a rocket exhaust tends to be a strong function of temperature.

Within the framework of this analysis, the marked difference between the chemically inert (cold) flows and dissociation and recombination phenomena (higher temperature flows) can be formally regarded as contributing significantly to the acoustic propagation of the medium. From the initial computations in Section IV, this dependence upon the temperature and Mach number of the rocket exhaust becomes self-evident.

I. FORCING FUNCTION FOR FINITE AMPLITUDE PRESSURE WAVE GENERATION

A volume, V, is considered to consist of an acoustic medium in a stationary state in which a smaller volume, ν, is so imbedded that ν consists of a violently disturbed medium. While in V the entropy is a well-defined thermodynamic variable, the same is not true for the disturbed volume ν due to the nonequilibrium states. To circumvent this difficulty in a formalistic way, the pressure function is defined as being made up of scalar functions p_1 and p_2, the first relating only to isentropic changes in V, and the second describing the nonisentropic processes in ν. Note also that the velocity vector $\vec{u}$ vanishes identically in the volume V and exists only in ν.

From the equations of motions we have

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\partial u_j) = 0 \tag{1}$$

$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial xj} (\rho u_i u_j) = \frac{\partial}{\partial xj} (\sigma_{ij}) \tag{2}$$

$$\rho \frac{\partial e}{\partial t} + \rho u_j \frac{\partial e}{\partial x_j} = \sigma_{ij} \frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j} (k \frac{\partial T}{\partial x_j}) + Q$$

$$S = S(\rho, T) \tag{3}$$

where

x_i = cartesian space-variable component

t = time

ρ = density

u_i = cartesian velocity component

σ_{ij} = stress tensor

e = internal energy

T = temperature

Q = heat sources

S = (entropy)

For the case of a homogeneous and isotropic medium we have

$$\sigma_{ij} = - p \ \delta_{ij} + \frac{2}{3}\mu \ \Sigma_{kk} \ \delta_{ij} + \mu \ \Sigma_{ij} \tag{4}$$

where Σ_{ij} equals the strain rate, δ_{ij} equals the Kronecker δ, and μ equals the viscosity coefficient.

When the medium in question is not a function of temperature, then, (under thermodynamic equilibrium conditions) the energy equation is uncoupled from the remaining equations of motion, and mechanical conditions dominate its behavior. However, in the case of violent physical and chemical processes, this uncoupling of the equations of motion may lead to physically questionable results. In this formulation, when high-energy entropy production rates are considered, such uncoupling seems to be unwarranted.

Next, the continuity and momentum equations are combined into one wave equation form. Using the definition of the pressure function for the stationary and disturbed regions, the momentum equation becomes

$$\frac{\partial}{\partial t}(\rho u_i) + a^2 \frac{\partial \rho}{\partial x_i} = - \frac{\partial}{\partial x_j}(\rho u_i u_j) - \frac{\partial P_2}{\partial x_i} + \frac{\partial}{\partial x_j}(\psi_{ij}) \tag{5}$$

with

$$\psi_{ij} = \frac{2}{3}\mu \ \Sigma_{kk} \ \delta_{ij} + \mu \ \Sigma_{ij}$$

Now, by cross-differentiating the continuity and momentum equations with respect to t and x_i respectively, and by subtracting, the following will result:

$$\frac{\partial^2 \rho}{\partial t^2} - \frac{a^2 \partial^2 \rho}{\partial x_i \partial x_i} = \frac{\partial}{\partial x_i}\left\{\frac{\partial}{\partial x_i}(\rho u_i u_j) + \frac{\partial P_2}{\partial x_i} - \frac{\partial}{\partial x_j}(\psi_{ij})\right\} \tag{6}$$

Now let

$$\frac{\partial}{\partial x_j}(\rho u_i u_j) = u_i \frac{\partial}{\partial x_j}(\rho u_j) + (\rho u_j)\frac{\partial u_i}{\partial x_j} - \rho u_j \frac{\partial u_j}{\partial x_i} + \rho u_j \frac{\partial u_j}{\partial x_i}$$

where the two last identical terms cancel each other. Then, note that

$$\rho u_j \frac{\partial u_i}{\partial x_j} - \rho u_j \frac{\partial u_j}{\partial x_i} = \rho u_j \frac{\partial u_m}{\partial x_n}\left[\delta_{in}\ \delta_{jm} - \delta_{im}\ \delta_{jn}\right]$$

$$= - \rho \epsilon_{ijk}\ \epsilon_{nmk}\ u_j \frac{\partial u_m}{\partial x_n}$$

with ϵ_{ijk} being the alternating tensor. Note that in vectorial notation

$$- \rho \epsilon_{ijk}\ \epsilon_{nmk}\ u_j \frac{\partial u_m}{\partial x_n} = \rho(\vec{u} \times \vec{\zeta}) \tag{7}$$

can be written where

$\vec{u}$ = velocity vector

$\vec{\zeta}$ = vorticity vector

Again, for the nonisentropic region ν

$$\frac{\partial p_2}{\partial x_i} = \rho \frac{\partial h}{\partial x_i} - T \frac{\partial S}{\partial x_i} \tag{8}$$

in which h equals enthalpy. Under these conditions, the wave equation in equation (6) becomes

$$\frac{\partial^2 \rho}{\partial t^3} - a^2 \frac{\partial^2 \rho}{\partial x_i \partial x_i} = \frac{\partial}{\partial x_i}\left\{- \rho \epsilon_{ijk}\ \epsilon_{nmk}\ u_j \frac{\partial u_m}{\partial x_n} + \rho\left(\frac{\partial h_o}{\partial x_i} - T \frac{\partial S}{\partial x_i}\right) + \frac{\partial}{\partial x_i}(\psi_{ij}) - u_i \frac{\partial \rho}{\partial t}\right\} \tag{9}$$

Here, $h_o = h + \frac{1}{2} u_i u_i$ refers to total enthalpy. In vectorial form this becomes

$$\frac{\partial^2 \rho}{\partial t^2} - a^2\nabla^2 \rho = \nabla \left\{ - \rho \vec{u} \times \vec{\zeta} + \rho (\Delta h_o - T\nabla S) + \vec{F}_i - \vec{u} \frac{\partial \rho}{\partial t} \right\} \tag{10}$$

where $\vec{F}_i = \frac{\partial}{\partial x_j} (\psi_{ij})$ represents the viscous terms. Equation (10), therefore, represents the required relation.

This equation is now formally simplified by focusing attention on entropy production regions. In this case, note that the total enthalpy terms representing the stagnation temperature remain constant even when crossing a shock wave. Since this would correspond to the highest entropy jump in the case of a supersonic rocket exhaust, this term may conceivably be disregarded.

In a formalistic manner, the viscous term may also be looked on as contributing to the entropy production gradient through the energy equation, since, in the absence of heat transfer and heat sources

$$\rho T \frac{dS}{dt} = \phi \tag{11}$$

where ϕ is the dissipation function, governed by viscosity.

Thus, the following equation is obtained:

$$\frac{\partial^2 \rho}{\partial t^2} - a^2\nabla^2 \rho = - \nabla \left\{ \vec{f} + \rho T \nabla S \right\} \tag{12}$$

$$. \ \vec{f} = (\rho \vec{u} \times \vec{\zeta} - u \frac{\partial \rho}{\partial t}$$

where the function $\vec{f}$ in the forcing function represents the contribution of density gradient and vorticity, and the second $\rho T \nabla S$ represents entropy production gradients coupled with the temperature and density functions.

For the case of highly supersonic flow, attention is concentrated on the shock layer regions where the entropy jump seems to be the greatest contributing factor. In any case, the generating function for the equation can be written in the form

$$G = - \frac{1}{4\pi a^2} \iiint \frac{1}{r} \nabla \left\{ \vec{f} + \rho \ T \nabla S \right\} dV \tag{13}$$

where the integral is taken over the disturbance region, and the retarded potential solution is implied.

It should be noted that this formalistic derivation holds true when the dependent variables (i.e., the physical processes) are continuous up to and including second derivatives. Thus, shock-layer conditions may be considered in the neighborhood of the shock wave but not in the shock itself. It follows that the contribution of the jump conditions must be treated as a special case.

It is also apparent that the unknown forcing function cannot be found from equation (13), and that, for its properties and variations in the neighborhood of a shock layer, available solutions in fluid flow theories must be utilized to apply them to the case of variable distributions in a highly hypersonic rocket exhaust. Thus, use is made of the available solutions in which the properties of these unknown functions are coupled intrinsically with the energy equation to obtain a physical picture of the regions considered.

II. THREE-DIMENSIONAL HYPERSONIC ENTROPY PRODUCTION[1]

In this section consideration is given to the investigation of conditions governing entropy production in regions adjacent to the shock layer, when the angle of inclination of the wave is small with respect to the stream direction at infinity. The partial differential equations governing the nonlinear axis-symmetric flows are given by

$$\frac{\partial \rho}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r}(\rho u r) = g\left(u_1, \frac{\partial u_1}{\partial x}\right)$$

$$\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial r} \quad \frac{1}{\rho}\frac{\partial p}{\partial r} = g'\left(u_1, \frac{\partial u_1}{\partial x}\right) \tag{14}$$

$$\frac{\partial s}{\partial t} + v\frac{\partial s}{\partial r} = g''\left(u_1, \frac{\partial u_1}{\partial x}\right)$$

with the boundary conditions behind the shock y_s being given by

$$\frac{p_s}{p_0} = \frac{2\gamma}{\gamma+1}\left(\frac{1}{a^2}\right)\frac{dy_s}{dt} - \frac{\gamma-1}{\gamma+1}$$

$$\frac{p_s}{p_0} = \frac{\gamma-1}{\gamma+1} + \frac{2}{\gamma+1} \; a^2/\left(\frac{dy_s}{dt}\right)^2 \tag{15}$$

$$V_s = \frac{2}{\gamma+1}\frac{dy_s}{dt}\left(1 - a^2/\left(\frac{dy_s}{dt}\right)^2\right)$$

The terms g, g', and g'' on the right-hand side of equations (14) are of second-order magnitude and can be neglected in accordance with the hypersonic disturbance theory behind the shock wave.

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[1] Based upon References 1 through 5.

For a strong shock, the boundary conditions may be reduced by omitting the terms of order $a^2/\left(\frac{dy_s}{dt}\right)^2$ to result in

$$p_s = \frac{2}{\gamma - 1}\,\rho_0\left(\frac{dy_s}{dt}\right)^2;\; \rho_s = \frac{\gamma + 1}{\gamma - 1}\,\rho_0;\; V_s = \frac{2}{\gamma + 1}\left(\frac{dy_s}{dt}\right)$$

By introducing a transformation of variables

$$P = \frac{p}{p_s};\; R = \frac{\rho}{\rho_s};\; V = \frac{v}{v_s};\; \eta = \frac{r}{y_s} \tag{16}$$

and by anticipating a self-similar solution, it is assumed that

$$p = p_s\,P_{(\eta)};\; \rho = \rho_s\,R_{(\eta)}\; v = v_s\,V_{(\eta)} \tag{17}$$

as a consequence of which we obtain, from equations (14)

$$\left(\frac{y_s\ddot{y}}{\dot{y}_s^{\,2}}\right)V + \left[\frac{2}{\gamma+1}V - \eta\right]V' = -\frac{\gamma-1}{\gamma+1}\,\frac{P'}{R}$$

$$2\left(\frac{y_s\ddot{y}_s}{\dot{y}_s^{\,2}}\right) + \left[\frac{2}{\gamma+1}V - \eta\right]\left[\frac{P'}{P} - \gamma\,\frac{R'}{R}\right] = 0 \tag{18}$$

$$\left[\frac{2}{\gamma+1}V - \eta\right]R' + \frac{2}{\gamma+1}R\left[V' + \frac{V}{\eta}\right] = 0$$

where the prime and dots signify derivatives with respect to η and t, respectively. For a self-similar solution to exist, the time dependent terms must be a constant. This calls for the shock-layer equation corresponding to a power-law $y_s \sim X\sigma$. Once the exponent σ is specified, P, R, and V are determined completely from the equations

$$\left[V - \frac{\gamma + 1}{2}\eta\right] \frac{V'}{V} + \frac{\gamma - 1}{2}\frac{P'}{RV} - \frac{1 - \sigma}{\sigma}\;\frac{\gamma + 1}{2} = 0$$

$$\left[V - \frac{\gamma + 1}{2}\eta\right] \left[\frac{P'}{P} - \frac{\gamma R'}{R}\right] - (\gamma + 1)\left(\frac{1 - \sigma}{\sigma}\right) = 0 \qquad (19)$$

$$\left[V - \frac{\gamma + 1}{2}\eta\right] \frac{R'}{R} + V' + V/\eta = 0$$

with the boundary conditions $P(1) = R(1) = V(1) = 1$ at $\eta = 1$. Except in a few cases, an explicit solution to the problem cannot be obtained. Numerical integration must be carried out inward from the shock at $\eta = 1$.

The investigation of solutions indicates that, close to the axis of symmetry, the entropy tends to infinity, whereas the pressure is finite. This is because, in the neighborhood of the axis, the gas has passed through a much stronger part of the shock wave (Mach disc) at an earlier time and thus has gained a much higher entropy. Since, to this approximation, the entropy function is conserved on the streamline (except at the shock transition where it takes a large jump), this higher entropy gain persists and is carried by the fluid particles along their paths. Because of the much higher entropy, the temperature in layers near the axis must be very high and the density very low, since the pressure there is finite. Thus, due to low density, the fluid acceleration produces negligible pressure gradients. Consequently, the pressure remains quite uniform throughout the layer.

The numerical integration of equations (18) which points to the presence of the entropy layer cannot be extended to the analysis of this layer since it is generated by almost normal shock conditions in the neighborhood of flow axis (blast wave analogy with no body present). Thus, the conditions of strong, blunt, shock layers, with the consequent high-entropy production, must be treated in a separate manner.

III. REFLECTION PROPERTIES OF PRESSURE WAVES

The determination of flow properties and entropy production rates in a supersonic rocket exhaust for chemically inert flows (using the method of characteristics and the equations of continuum mechanics exclusively), in the form of an explicit approximate expression in the forcing function of the nonlinear wave equation, calls for knowledge of the shock-layer shape forming in the wake of the underexpanded nozzle. The reflection properties of the pressure waves formed in the exhaust gas and emanating from a supersonic axisymmetric nozzle can be studied to a high degree of approximation by the numerical methods of characteristics.

In this formulation, the method of characteristics has been utilized to investigate the reflection patterns of the pressure waves from the free boundaries. Special emphasis has been placed upon determining the coalescence pattern of pressure waves after reflection from the free boundary has taken place. This approach allows for the analytical numerical tracing of the intercepting shock patterns to be approximated at a later stage, if so desired, by an analytical expression, based upon numerical results.

The physical considerations of the phenomena are as follows. As the gas accelerates from the sonic condition at the throat of the nozzle, expansion fans are formed and those fans directed outward and upward strike the jet boundary. Since this is basically a free boundary, the expansion fans reflect from it in the opposite sense and become compression waves. Moreover, due to the convex form of the free boundary, these compression waves eventually coalesce into a plume shock layer. The computations have been carried out for very high pressure ratios to accentuate the effect; but the method remains identical for all higher than critical pressure ratios, and extension to lower pressure ratios is immediate.

The computations are based upon a cylindrical coordinate system (i.e., x, r) where the x axis is coincident with the axis of symmetry of the flow and, if P and ρ indicate pressure and density in addition to u and v (the velocity components along the x and r axes respectively), Euler's equations are given by

$$u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial r} = - \frac{1}{\rho} \frac{\partial P}{\partial x}$$
$$u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial r} = - \frac{1}{\rho} \frac{\partial P}{\partial r} \tag{20}$$

and the equation of continuity is

$$\frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial r} + \frac{\rho v}{r} = 0 \tag{21}$$

The total enthalpy, h_T, is constant along each streamline and the equation

$$u \frac{\partial h_T}{\partial x} + v \frac{\partial h_T}{\partial r} = 0 \tag{22}$$

is valid everywhere, while the entropy, s, is represented by the equation

$$u \frac{\partial s}{\partial x} + v \frac{\partial s}{\partial r} = 0 \tag{23}$$

and is valid everywhere except for passage through a shock wave.

The velocity of sound, C, for the general case along a streamline is given by

$$C = \left(\sqrt{\frac{\partial P}{\partial \rho}}\right)_{s=const} = \sqrt{\frac{\partial P}{\partial \rho}} = \sqrt{\gamma RT} \tag{24}$$

The relation between pressure and density in an ideal gas having C_p and C_v constant is given by

$$\frac{P}{\rho^\gamma} = \frac{P_i}{\rho_i^\gamma} e^{\frac{s-s_i}{C_v}} = C e^{\frac{s}{C_v}} \tag{25}$$

where P_i, ρ_i, and s_i are the initial conditions and $\gamma = C_p/C_v$. Because of equations (22) and (23), the initial conditions and, therefore, C remain constant along each streamline. From equations (24) and (25) the following relations are obtained

$$\frac{\partial P}{\partial x} = \rho \frac{C^2}{Cp} \frac{\partial s}{\partial x} + C^2 \frac{\partial \rho}{\partial x} + \rho \frac{C^2}{\gamma} \frac{\partial \ln C}{\partial x} \tag{26}$$

$$\frac{\partial P}{\partial y} = \rho \frac{C^2}{Cp} \frac{\partial s}{\partial r} + C^2 \frac{\partial p}{\partial r} + \rho \frac{C^2}{\gamma} \frac{\partial \ln C}{\partial r} \tag{27}$$

The relationships among entropy, total enthalpy, and vorticity component normal to the streamline for axially symmetric flow are given by

$$(\vec{v} \times \text{curl } \vec{v}) \circ \vec{n} = - v \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial r} \right) \tag{28}$$

and, therefore,

$$\frac{\partial v}{\partial x} - \frac{\partial u}{\partial r} = - \frac{1}{v} \frac{\partial h_T}{\partial n} + \frac{C^2}{\gamma R v} \frac{\partial s}{\partial n} \tag{29}$$

By combining equations (20) to (24), (26) and (27) the expression

$$\frac{\partial u}{\partial x} \left(1 - \frac{u^2}{C^2} \right) + \frac{\partial v}{\partial r} \left(1 - \frac{v^2}{C^2} \right) - \frac{uv}{C^2} \left(\frac{\partial u}{\partial r} + \frac{\partial v}{\partial x} \right) + \frac{v}{r} = 0 \tag{30}$$

is obtained. It is convenient at this point to define the functions

$$\psi_x = - rv \, (1-w^2)^{\frac{1}{\gamma - 1}} \tag{31}$$

$$\psi_r = ru \, (1-w^2)^{\frac{1}{\gamma - 1}} \tag{32}$$

$$f(\psi) = \frac{v_x - u_r}{r(1-w^2)^{\frac{\gamma}{\gamma - 1}}} \tag{33}$$

with $w = v/v_l$, i.e., ratio of the local velocity to limiting velocity. Utilizing equations (31), (32), and (33), equation (30) can be put into the following form

$$\left(1 - \frac{u^2}{C^2} \right) \psi_{xx} - \frac{2uv}{C^2} \psi_{xr} + \left(1 - \frac{v^2}{C^2} \right) \psi_{rr} - \frac{\psi_r}{r} - r^2 (1-w^2)^{\frac{\gamma+1}{\gamma-1}} \left(\frac{w^2}{C^2} - 1 \right) f(\psi) = 0 \tag{34}$$

Following the procedure of Ferri (References 6 and 7), we define

$$H = 1 - u^2/C^2 \tag{35}$$

$$L = 1 - v^2/C^2 \tag{36}$$

$$K = \quad - uv/C^2 \tag{37}$$

and,

$$N = -\frac{\psi_r}{r} - r^2(1-w^2)^{\frac{\gamma+1}{\gamma-1}} \left(\frac{w^2}{C^2}\right) - 1 \quad f(\psi)$$

Thus, equation (34) may be written

$$H\psi_{xx} + 2K\psi_{xr} + L\psi_{rr} + N = 0 \tag{38}$$

and

$$\frac{d\psi_x}{dx} = \psi_{xx} + \psi_{xr}\frac{dr}{dx} \tag{39}$$

$$\frac{d\psi_r}{dx} = \psi_{xr} + \psi_{rr}\frac{dr}{dx} \tag{40}$$

The simultaneous solution of equations (38) through (40) will yield

$$\left(\frac{dr}{dx}\right)_{I,II} = \frac{K}{H} \pm \sqrt{+\frac{K^2}{H^2} - \frac{L}{H}} \tag{41}$$

$$\psi_{xx} + \left(\frac{K}{H} \pm \sqrt{\frac{K^2}{H^2} - \frac{L}{H}}\right)\psi_{xr} + \frac{N}{H} = 0 \tag{42}$$

Upon substitution of

$$u = V \cos\theta \tag{43}$$

$$S = V \sin\theta \tag{44}$$

$$C = V \sin\mu \tag{45}$$

equation (41) transforms to

$$\left(\frac{dr}{dx}\right)_{I,II} = \tan(\theta \pm \mu) \tag{46}$$

The positive sign refers to the first family or left-running characteristics, whereas the negative sign refers to the second family or right-running characteristics.

Equation (42) combined with equation (31) and the vorticity relation

$$\frac{(\text{curl } \vec{v}) \times \vec{V}}{c} = \frac{1}{\gamma R} \text{ Grad } S = \frac{1}{\gamma R} \frac{ds}{dn} \tag{47}$$

yield

$$\frac{dW}{W} \pm \tan\mu \, d\theta - \frac{\text{Sin}\,\mu \ \text{Sin}\,\theta \ \tan\mu}{\text{Cos}\,(\theta \pm \mu)} \frac{dx}{r} \pm \frac{\text{Sin}^3\mu}{\text{Cos}(\theta \pm \mu)} \frac{dx}{dn} \frac{S}{\gamma R} = 0 \tag{48}$$

The Mach number is a more convenient parameter than the nondimensional velocity ratio W; therefore

$$\frac{dW}{W} = \frac{dV}{V} = \frac{dM}{M\left(1 + \frac{\gamma - 1}{2} M^2\right)} \tag{49}$$

and equation (48) transforms into

$$\frac{dM}{\left(1 + \frac{\gamma-1}{2} M^2\right) M \tan\mu} \pm d\theta - \frac{\text{Sin}\,\mu \ \text{Sin}\,\theta}{\text{Cos}\,(\theta \pm \mu)} \frac{dx}{r} \pm \frac{\text{Sin}^3\,\mu}{\tan\mu \ \text{Cos}\,(\theta \pm \mu)} \frac{S}{\gamma R} \frac{dx}{dn} = 0 \tag{50}$$

Now, since

$$\begin{aligned} \text{Sin}\,\mu &= \frac{1}{M} \\ \text{Cos}\,\mu &= \frac{\sqrt{M^2 - 1}}{M} \\ \tan\mu &= \frac{1}{\sqrt{M^2 - 1}} \end{aligned} \tag{51}$$

(Equation 51 cont next page.)

$$C_p = \frac{\gamma R}{\gamma - 1}$$
$$\left(\frac{dx}{dn}\right)_{I,II} = \frac{\text{Cos }(\theta \pm \mu)}{\text{Sin}} \tag{51}$$

and, therefore, equation (50) becomes

$$\frac{\sqrt{M^2 - 1}\ dM}{\left(1 + \frac{\gamma - 1}{2} M^2\right) M} \pm d\theta - \frac{dx}{(\sqrt{M^2 - 1}\ \text{Cot}\,\theta \pm 1)^2} \pm \frac{\sqrt{M^2 - 1}\ ds}{(\gamma - 1)\ M^2} = 0 \tag{52}$$

Following the nomenclature of Reference (8), equations (46) and (52) may be expressed in finite difference form. For the first family or left-running characteristic,

$$\Delta\theta = A\Delta M - B\Delta x + C\Delta S \tag{53}$$

$$\Delta r = \Delta x / K \tag{54}$$

For the second family or right-running characteristic,

$$\Delta\theta = -A\Delta M + b\Delta x - C\Delta S \tag{55}$$

$$\Delta r = \lambda \Delta x. \tag{56}$$

The preceding formulation defines the general scheme of the procedure undertaken to analyze reflection properties of pressure waves in the exhaust nozzle, based upon finite difference methods. Further details are based upon References 8, 9 and 10. However, specific mention of the procedure of applying Prandtl-Mayer flows to the corner regions of the nozzle will be made.

If equation (39) is employed to compute the flow conditions in the immediate vicinity of a sharp corner, e.g., the lip of the nozzle, the terms containing dx and ds vanish and equation (52) reduces to

$$\pm d\theta = \frac{\sqrt{M^2 - 1}}{M\left(1 + \frac{\gamma - 1}{2} M^2\right)} dM \tag{57}$$

and, upon integration, yields

$$\pm \theta = \sqrt{\frac{\gamma + 1}{\gamma - 1}} \tan^{-1} \sqrt{\frac{\gamma - 1}{\gamma + 1} (M^2 - 1)} - \tan^{-1} \sqrt{M^2 - 1} + \text{Const} \tag{58}$$

Now, the Prandtl-Meyer angle (ν), through which the stream turns in expanding from a sonic condition to a supersonic Mach number, is

$$\nu = \sqrt{\frac{\gamma+1}{\gamma-1}} \tan^{-1}\sqrt{\frac{\gamma-1}{\gamma+1}(M^2-1)} - \tan^{-1}\sqrt{M^2-1} \tag{59}$$

Corner type flow occurs in the vicinity of the nozzle lip (Figure 1), and the amount of turning is determined by the initial and final Mach number at the nozzle lip. The final Mach number is determined from the ratio of the ambient to total chamber pressure; and since, for isentropic flow, this pressure ratio is directly a function of the final Mach number, γ, it can be expressed as

$$\frac{P_b}{P_T} = \left(1 + \frac{\gamma-1}{2} M^2\right)^{-\frac{\gamma}{\gamma-1}} \tag{60}$$

Equation (59) also indicates that ν is a function of the Mach number. Therefore, knowledge of the pressure ratio is equivalent to knowledge of the final ν and, hence, knowledge of the total turning angle of the flow around the nozzle lip. The boundary Mach number becomes infinitely large as the

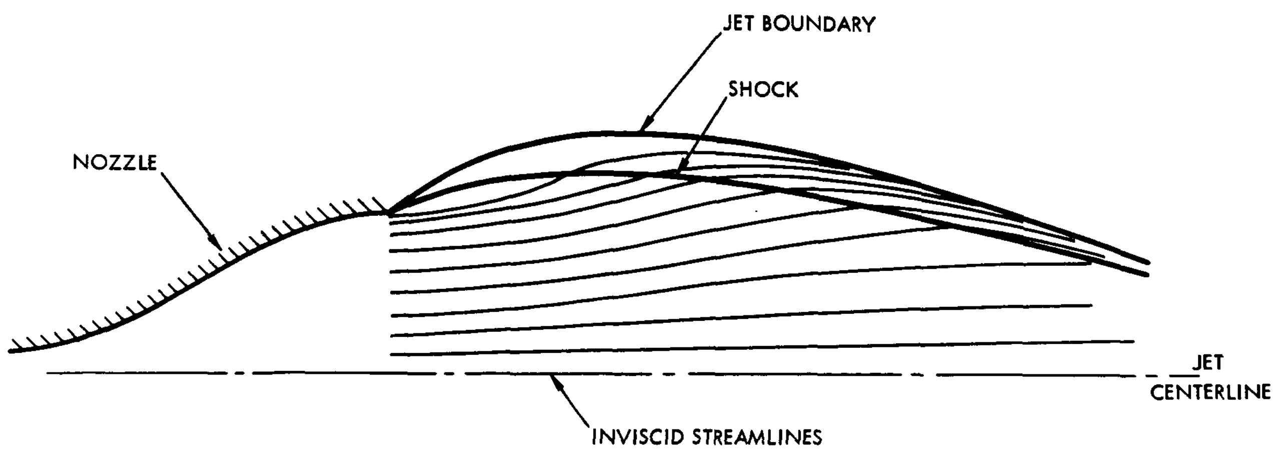


Figure 1. Physical Characteristics of the Primary Wavelength of a Supersonic Jet from a Contoured Nozzle

boundary pressure is reduced; in this case, the Prandtl-Meyer angle corresponding to the boundary Mach number would approach the maximum value of ν defined by

$$\nu_{MAX} = \left(\sqrt{\frac{\gamma+1}{\gamma-1}} - 1\right)\frac{\pi}{2} \tag{61}$$

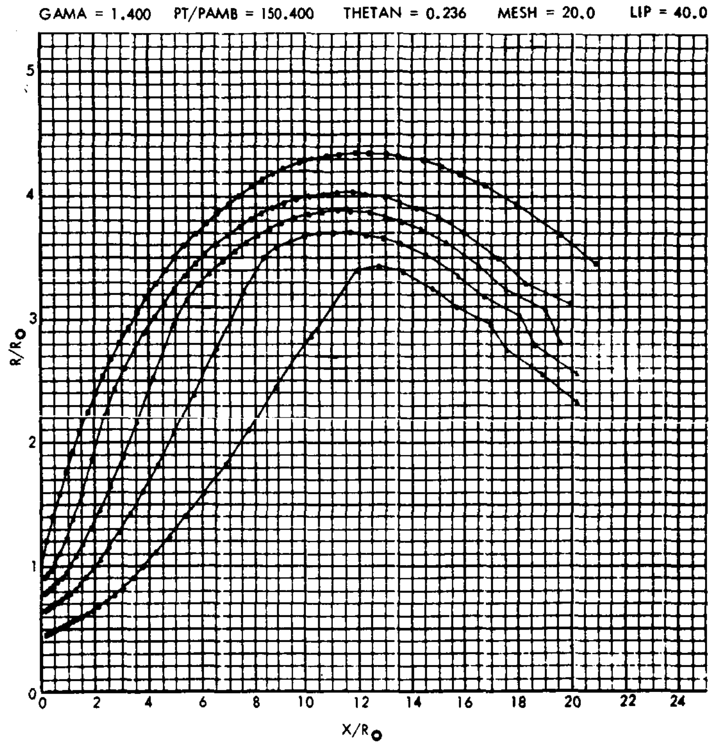
At very low or very high temperatures and pressures, the assumption of an ideal continuum fluid is not likely to be valid; however, the results may be used as a guide.

It is noted from the results of this analysis that, as the pressure ratios tend to infinity (Figure 2) the angle between the nozzle tip and the jet boundary grows to such an extent that a flow reversal phenomenon is encountered. The approach includes provisions for rotational flow, of primary importance in entropy generation. The internal nozzle flow has not been considered: even when the nozzle is contoured to provide an isentropic expansion, entropy charges are accounted for in the region bounded by the plume. These charges are a consequence of the presence of vorticity and are also due to the Rankine-Hugoniot jump conditions across the shock.

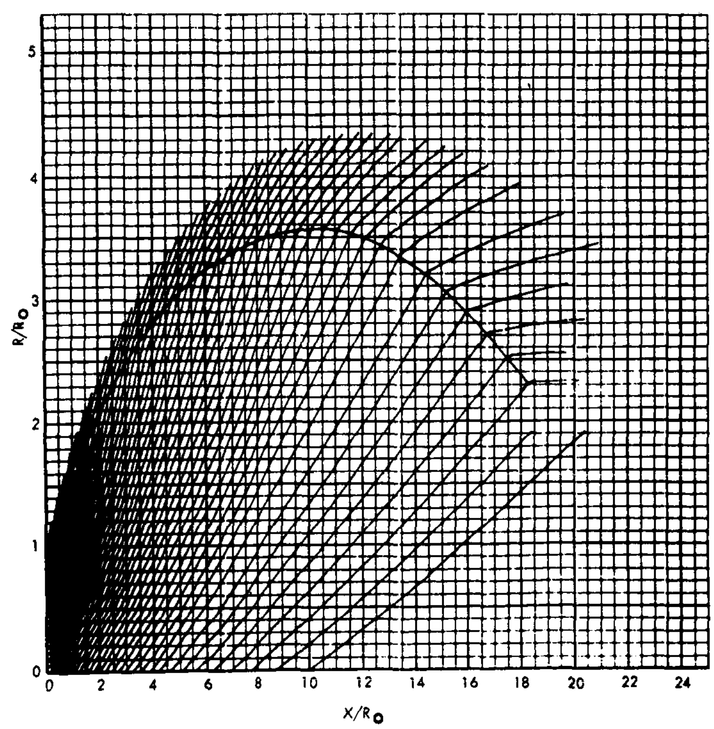
The characteristic solution was programmed for the IBM 7090 computer with provisions to obtain cathode-ray tube (CRT) plotting of the characteristics, streamlines, and constant Mach lines. The computations were carried out along left-running characteristics, starting at the nozzle tip. The number of divisions at the nozzle exit and tip is directly a function of the accuracy desired. Provisions were also made to increase the number of divisions in the flow field to compensate for the divergence of the original characteristics as the tendency of divergence increases.

The applicability of the characteristic solution is limited to the appearance of the Mach disc in the flow which cannot be accounted for from the present formulation; however, the linear theory provides a guide to the applicable range of the solution, since it calls for the diameter of the jet at the primary wave length to be equal to the nozzle diameter. This condition, therefore, provides a limit of the applicability of the solution, and it determines the extent of downstream validity of the characteristic plot before the subsonic region behind the Mach disc is reached.

The region of entropy production in the wake of the rocket exhaust for high pressure ratios obtained from the aforementioned characteristic solution has been programmed with provisions to obtain CRT presentation of the characteristics, streamlines, and constant Mach number lines.



VIEW A. STREAMLINES



VIEW B. CHARACTERISTICS

Figure 2. CRT Plots of Streamlines and Left-Running Characteristics and Coalescence Points Forming the Shock (Sheet 1 of 4)

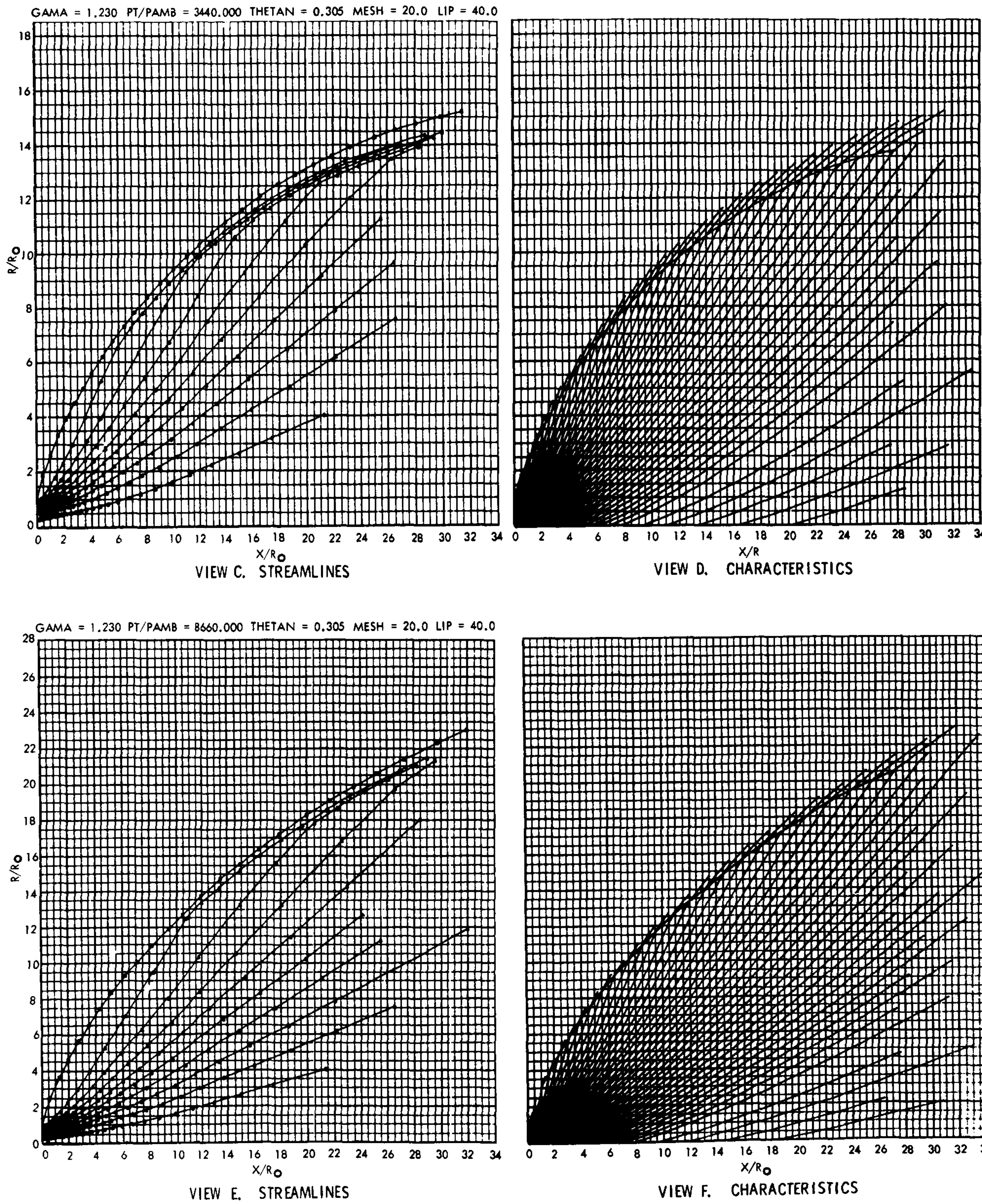


Figure 2. CRT Plots of Streamlines and Left-Running Characteristics and Coalescence Points Forming the Shock (Sheet 2 of 4)

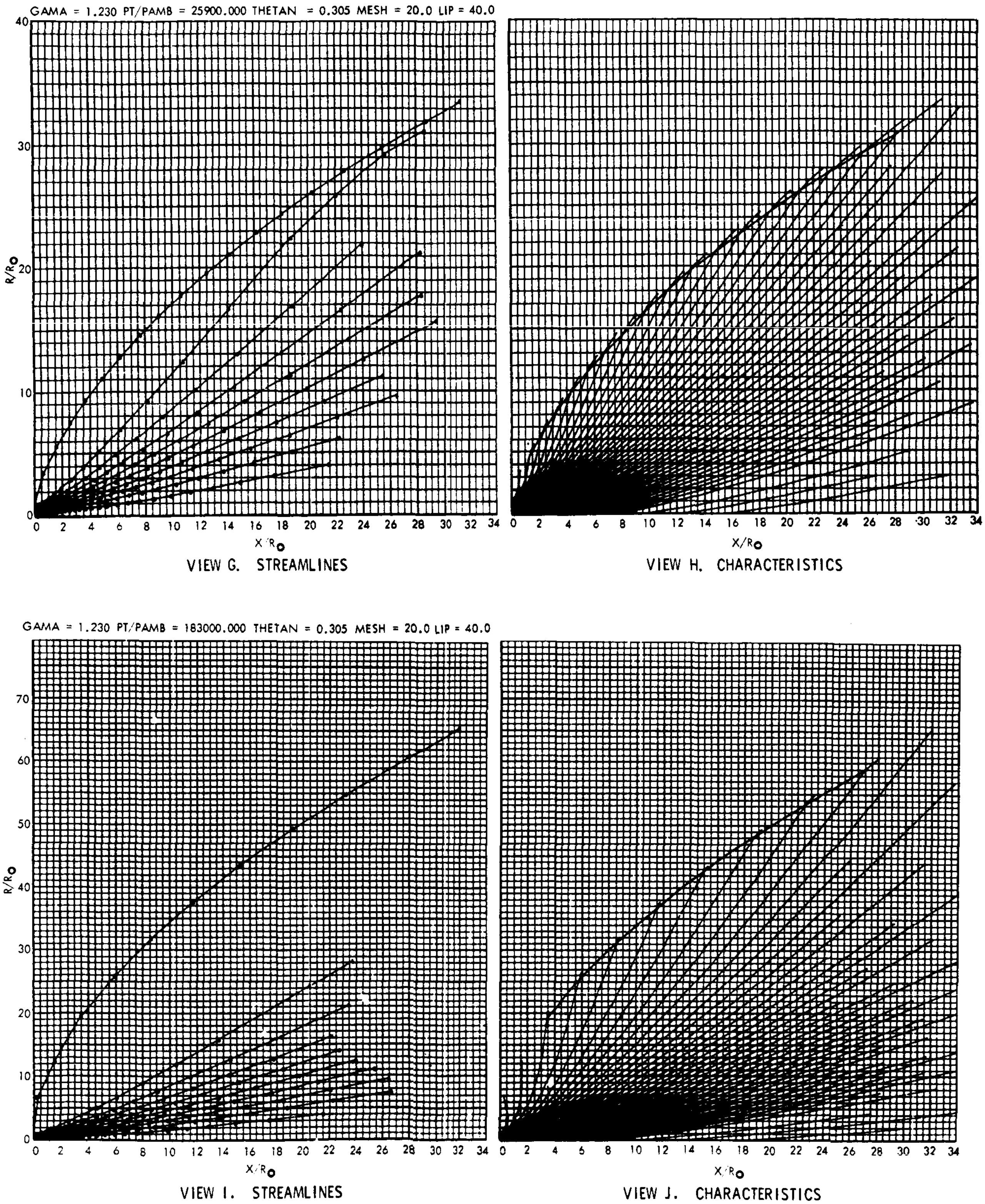


Figure 2. CRT Plots of Streamlines and Left-Running Characteristics and Coalescence Points Forming the Shock (Sheet 3 of 4)

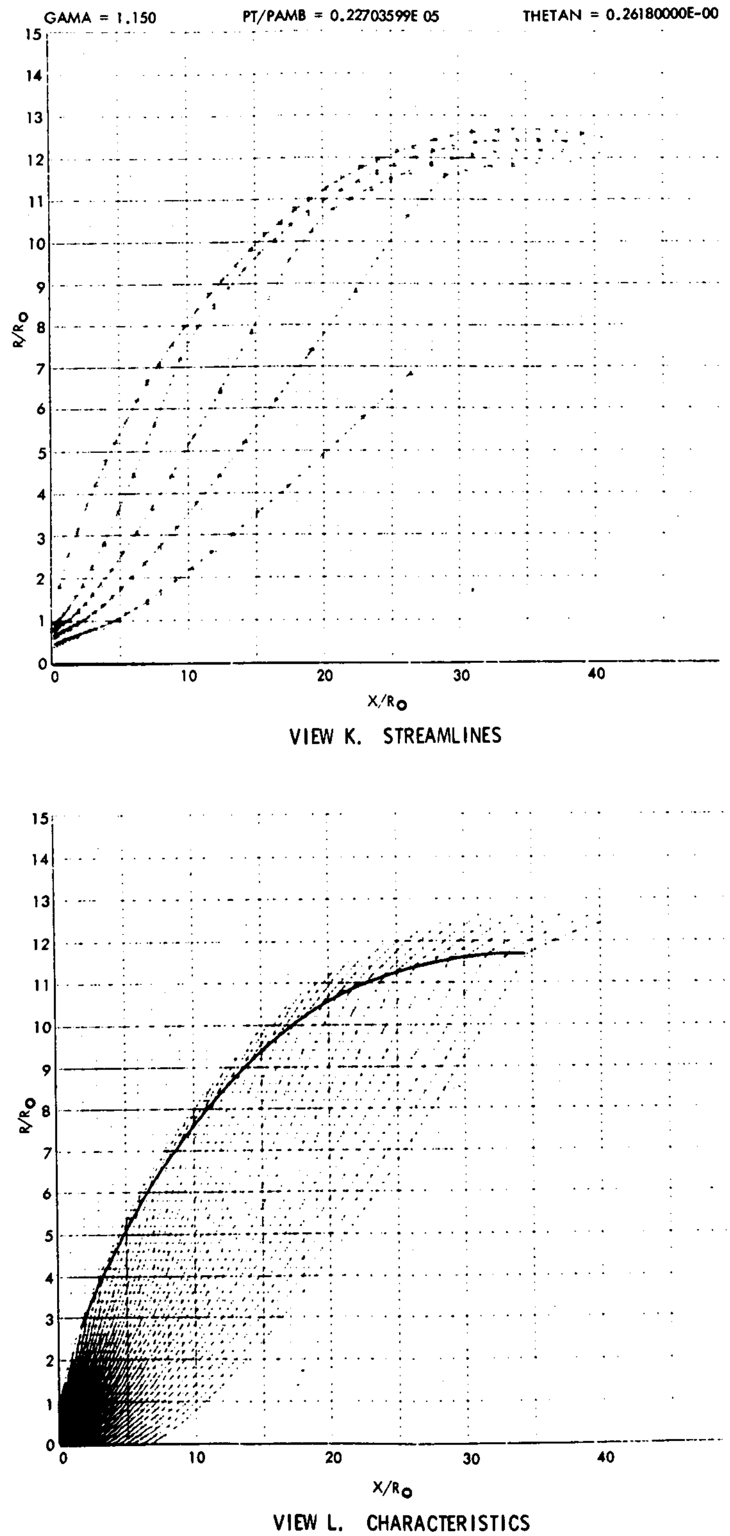


Figure 2. CRT Plots of Streamlines and Left-Running Characteristics and Coalescence Points Forming the Shock (Sheet 4 of 4)

Initial computations were functions of the choice of nozzle (i.e., for a conical nozzle, the nozzle spherical surface is chosen, whereas for a bell nozzle, the exit plane is utilized); however, any arbitrary right-running characteristic with known flow conditions may be used as an input to the program.

Assuming the nozzle exit conditions (e.g., x, r, M, θ, and s) are known, the exit plane is divided into an arbitrary number of equal parts, depending upon the accuracy desired. Through each such point, left- and right-running characteristics emanate. In the vicinity of the nozzle lip, corner-type flow prevails and the initial and final Prandtl-Meyer angle may be computed; this, in turn, is divided into a number of equal parts for use in the program.

Examples of the type of solutions of programmed analysis have been computed. The present results have been obtained using the weak shock assumption. CRT plots of streamlines and corresponding left-running characteristics as functions of R/R_o and x/x_o are shown in Figure 2 for various free stream conditions. The data listed at the top of each streamline plot indicate the conditions under which the case was computed. For convenience, the nomenclature is defined here as follows:

GAMA -- Ratio of specific heats

PT/PAMB -- Ratio of jet total pressure to free stream ambient pressure

THETAN -- Angle of nozzle lip measured from horizontal in radians

MESH -- Imposed grid size on radius of nozzle

LIP -- Imposed divisions on total turning angle

Investigations regarding the Mach disk and second Mach diamond are logical extensions of the present analysis which may be used as a basis for a secondary approach in the vicinity of the subsonic segment of the flow since, in this region, the present approach of the method of characteristics does not apply.

Some considerations of the flow behind the Mach discs and their entropy productions for the case of chemically inert (cold) flows and chemically reacting (high-temperature) flows are given in the next section of this report.

IV. CHEMICALLY REACTING FLOWS

FLOW CHEMISTRY IN HYPERSONIC SHOCK LAYERS FOR NONEQUILIBRIUM GAS DYNAMICS[1]

In the presence of strong shock waves in hypersonic flow, the dissociation of gas molecules often occurs and makes a marked contribution to entropy production in the shock region. In addition, the nonequilibrium state of the gas is often carried along the streamline into the flow field behind the shock, causing the chemical nonequilibrium conditions to persist in the flow region. A short summary of the basic thermodynamic principles of these phenomena is presented in this section as a contribution to higher entropy production through collision phenomena and a consequent chemical flow instability which may contribute to aerodynamic sound generation.

The thermodynamic state of a gas mixture at a point in a nonuniform, unsteady field is determined completely by the local values of the two variables p and T, or ρ and T, if all internal processes take place rapidly (i.e., if the relaxation time is short), in which case, the thermodynamic equilibrium is attained locally. The rate of approach to local equilibrium varies, depending on the molecular and atomic structure and the processes involved. For a specified time scale in particular, thermodynamic equilibrium may not be fully established.

In many gas dynamics problems, thermodynamic equilibrium time can be considerably larger than the reciprocal of the mean of the collision frequency of the gas particle for the translational degree of freedom. In this case, it is possible to treat each component in different internal states as an isolated thermodynamic system whose exchange of energy with the other systems is slow. Such a treatment can be carried out, however, only if the equations specifying the rate of exchange, excitation, or de-excitation of the internal processes are fully known. Nevertheless, the rates associated with the excitation and de-excitation processes of a molecular rotation, vibration, dissociation (in air, dissociation involves not only the simple decomposition and recombination of the oxygen and nitrogen molecule, but also the formation of NO and other components), and ionization differ so widely that it may be possible to treat the principal nonequilibrium processes one at a time.

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[1] Based upon References 1, 3, 6, 7, 8, and 9.

In most works on flow chemistry, the rotational, vibrational, and electronic states of the atom and molecule are assumed to be in equilibrium at the translational temperature T. This assumption is adopted here.

The mass fraction of each gas species i is represented by C_i. Considering only chemical nonequilibrium, the thermodynamic state of the gas may be specified by the variables p, T, and C_i s. Of course, to distinguish the gas sample completely, the initial values of these variables must also be specified.

By definition

$$C_i = m_i n_i, \ \sum_i C_i = 1, \ \sum_i n_i = n, \ \rho = \sum_i m_i n_i \tag{62}$$

where n_i is the number fraction of the species i, and m_i is the mass per particle of the species i.

The equation of state for a perfect gas is

$$P = nkT = \sum_i p_i = \rho T \sum_i R_i C_i \tag{63}$$

where p_i is the partial pressure. Also

$$R_i = \frac{\mathcal{R}}{M} \tag{64}$$

where M is the molecular weight and $\mathcal{R}$ the universal gas constant, ($\mathcal{R}$ equals 1.98717 cal/mole-°K).

The specific internal energy of the gas is

$$e = \sum_i C_i e_i \tag{65}$$

with

$$e_i - e_{i_0} = \int_0^T (C_v)_i \, dT \tag{66}$$

where $(C_v)_{i_0}$ is the heat of formation per unit mass of the species (at absolute zero), and $(C_v)_i$ is the specific heat of that species at constant volume. Thus, by definition $(C_v)_i$ does not include heat of formation.

And now

$$h_i = \int_o^T C_{p_i} \, dT + (h_i)_o \tag{67}$$

Note that $(h_i)_o$ equals $(e_i)_o$ and that e_i and h_i are functions of temperature, T, alone, since each species, taken by itself, is a caloric perfect gas.

Since each component of the mixture considered has a uniform temperature and pressure and the processes of exchange with other systems are slow, there exists an entropy function S_i:

$$T \, dS_i = de_i + p_i \, d\left(\frac{1}{\rho_i}\right) \tag{68}$$

According to Gibbs, a specific entropy for the mixture can be defined as

$$S = \sum_i C_i S_i \, (p_i, T) \tag{69}$$

which is completely specified by p, T, and C_i. This definition of entropy is not generally the same as the ordinary one used in thermodynamics; i.e.,

$$S_E = \int_{PATH} \frac{dQ}{T} \tag{70}$$

which can be defined by p, T, and C_i only for a gas in full thermodynamic equilibrium since the integrals depend on the path. Thus, only in full equilibrium does

$$S_E = S \tag{71}$$

Moreover, in full thermodynamic equilibrium, there exists a free energy, F, and the thermodynamic potential function, G, so that

$$\begin{aligned} F &= E - TS \\ G &= H - TS \end{aligned} \tag{72}$$

The second law of thermodynamics is that for any process with volume and temperature fixed $\delta F \geq 0$. Alternatively, with p and T fixed $\delta G \geq 0$.

The stoichiometric equations $2H_2 + O_2 \rightleftarrows 2H_2O$, $2N \rightleftarrows N_2$, etc., may be generalized into the form

$$\sum_i \nu_i^{(j)} A_i \rightleftarrows 0 \tag{73}$$

where $\nu_i^{(j)}$ is the number of moles of the species A_i, which is required for the completion of the reaction. For example, in the equation

$$2H_2 + O_2 \rightleftarrows 2H_2O$$

$$\begin{aligned} \nu_1' &= 2 \; ; \; A_1 = H_2 \\ \nu_2' &= 1 \; ; \; A_2 = O_2 \\ \nu_3'' &= -2 \; ; \; A_3 = H_2O \end{aligned} \tag{74}$$

In equilibrium, the gas composition is determined completely by p and T. For each stoichiometric equation there is an equilibrium constant, K associated with the partial pressure, p_i, so that

$$\prod_i^N (p_i)^{\nu_i^{(j)}} = K(T) \tag{75}$$

which is only a function of T. There are as many equilibrium constants as stoichiometric equations. With the aid of the requirement that the total number of the same atomic species must be conserved in chemical reaction, the composition C_i, or the partial pressure p_i, can be completely determined. The fact that the root mean square of equation (10) is independent of p_i (the mass action law) may be anticipated from equation (8) which may be rewritten

$$\sum_{i=1}^{N_A} \nu_i' A_i \rightleftarrows \sum_{j=1}^{N_B} \nu_j'' B_j \tag{76}$$

where ν_i' and ν_j'' are now both positive integers, because in equilibrium the rate of conversion from A_i^S to B_i^S must balance that from B_i^S to A_i^S. The former is proportional to the probability of finding the reaction partners together; thus, it is proportional to $(B_j)^{\nu_j''}$. Similarly, the latter is proportional to $(p_i)^{\nu_i'}$, and it follows that K should be independent of the pressure.

The manner in which K depends on T can be deduced from classical thermodynamics. In practice, the absolute value of K can be most expediently computed in terms of the partition function in statistical mechanics, using partition functions determined separately for translation and rotation, vibration, and electronic excitation from the quantum atomic theory.

In the standard treatment of the equilibrium constant, the fact that for a specified volume and temperature, the free energy, F, attains a minimum in equilibrium ($\delta F \geq 0$), or alternatively that for a specified p and T, the potential G becomes a minimum in equilibrium ($\delta G \geq 0$) may be used. An alternative derivation of K (T) versus T may be obtained, based strictly on the assumption of equilibrium, and bypassing the use of the minimum principle and thus, the second law of thermodynamics.

The preceding statistical thermodynamic model allows one to take into account the nonequilibrium entropy production in regions where violent physical processes occur. It would seem only reasonable that, in the case of aerodynamic sound generation for rocket exhausts where strong shock waves of high intensity occur, these processes, which cannot be treated by means of continuum fluid mechanics alone, should be investigated.

CHEMICALLY REACTING GASES

When flow chemistry is taken into consideration, the dynamic behavior of any gas varies between an infinitely fast reaction (chemical equilibrium) and an infinitely slow reaction (chemically inert flows). It then follows that the nonequilibrium behavior of the gas will always be intermediate between these two extremes. In comparing entropy productions of chemically reacting flows in equilibrium to those of chemically inert flows, it is of special interest to consider the transition properties of the gas through a highly irreversible Mach disc of a rocket exhaust. This comparison should give indications of the difference in order of magnitudes of hot (reacting) and cold (nonreacting) flows as far as the entropy production through a Mach disc transition is concerned.

The following analysis of chemical flow kinetics (References 13 through 23), under the assumptions of a binary collision model (i.e., binary collision of atoms and molecules predominates and determines the thermodynamic gas state), is presented to give a qualitative picture and quantitative analysis of the contribution of chemically reacting flows to the entropy production where transition through a Mach disc of a rocket exhaust is concerned.

Assuming that the dissociation of the molecule, A_m, into two atoms, A_a, is caused by a collision between the molecule, A_m, and a second body, and that recombination follows a simultaneous encounter between two atoms, A_a, and the same second body, the stoichiometric equation describing the flow is given by the equation (Reference 20)

$$A_m + X \underset{K_r}{\overset{K_f}{\rightleftharpoons}} 2\,A_a + X \qquad (77)$$

where the quantity, X, denotes the second body.

For this reaction the stoichiometric coefficients are

$$\nu'_m = 1 \qquad \nu'_a = 0 \qquad \nu'_X = 1$$

$$\nu''_m = 0 \qquad \nu''_a = 2 \qquad \nu''_X = 1$$

where the ν_i are defined in relation 74.

Since the quantity, X, is not affected by the chemical reaction (Reference 20)

$$C_X = C_a + C_m = 1$$

$$2M_a = M_m$$

$$M_x = \frac{M_m}{1+C_a}$$

This follows from the fact that the molecular weight of X is the mean molecular weight of the mixture, namely, $M_m/(1+C_a)$.

The rate of production of the atomic species, $\dot{\omega}_a$, is given by (Reference 20)

$$\dot{\omega}_a = \frac{M_m}{t}\left[K\,(1-C_a) - C_a^2\right] \qquad (78)$$

where

$$t = \frac{M_m^3}{\left(4K_r\,\rho^2(1+C_a)\right)} \qquad (79)$$

$$K = \frac{\rho e}{\rho}\left[\frac{C_{ae}^2}{1-C_{ae}}\right] \qquad (80)$$

where subscript e refers the condition at chemical equilibrium.

For the ideal dissociating gas, the equilibrium composition, C_{ae}, is given by (Reference 17)

$$\frac{C_{ae}^{2}}{1-C_{ae}} = \frac{\rho d}{\rho_e} \exp\left[-\frac{Dm}{R_m T}\right] \quad (81)$$

where ρ_d equals the characteristic dissociation density which is constant for the ideal dissociating gas (Reference 17) and D_m equals the dissociation energy.

Comparison of equations (80) and (81) shows that

$$K = \frac{\rho_d}{\rho} \exp\left[-\frac{Dm}{R_m T}\right] \quad (82)$$

Substitution of equation (82) into equation (78) results in

$$\dot{\omega}_a = \frac{M_m}{t}\left[(1-C_a)\frac{\rho_d}{\rho} \exp\left[-\frac{Dm}{R_m T}\right] - C_a^2\right] \quad (83)$$

The species continuity equation for the atomic species may now be written in the form (Reference 20)

$$\rho_u \frac{dC_a}{dx} + \frac{d}{dx}(\rho C_a U_a) = \frac{M_m}{t}\left[(1-C_a)\rho d \exp\left[-\frac{Dm}{R_m T}\right] - C_a^2\right] \quad (84)$$

As mentioned previously, t may be interpreted as a characteristic reaction time with the following significance.

If the reaction occurs very rapidly, the value of C_a will differ only slightly from the local equilibrium value. In the limiting case, as t approaches zero, the bracket on the right-hand side of equation (84) must approach zero. The limiting case in which t is effectively zero (infinitely fast reactions) is called equilibrium flow, and the composition of the mixture is governed by equation (81).

For infinitely fast reaction, the dynamic behavior is very slow in comparison with the dissociation and recombination rates and results in a balance of the latter throughout the flow.

At the other limit, t may be so large (very slow reaction) that the rate of production, $\dot{\omega}_a$, is effectively zero. The gas may then be considered chemically inert and is usually referred to as a chemically frozen flow. In this case, the dynamic behavior of the gas is so rapid in comparison to the chemical changes that the latter exert little influence on the chemical composition of the gas mixture.

In any analysis of chemical nonequilibrium flow, the chief difficulties arise from the nonlinear coupling between the gas dynamic equations and the chemical relaxation equation. However, in the two extreme cases of frozen or equilibrium flow, the chemical relaxation equation is reduced to a very simple form, thereby simplifying the analysis.

GENERAL EQUATIONS OF CHANGE

The equations (Reference 20) governing the Mach disc (normal shock) transition of a mixture of atoms and molecules which behave individually as perfect gases, are as follows:

Mixture Continuity Equation

The mixture continuity equation

$$\frac{d(\rho u)}{dx} = 0 \tag{85}$$

which has the first integral

$$\rho u = (\rho u)_o = m = \text{constant} \tag{86}$$

Species Continuity Equation

The species continuity equation for the i^{th} species is

$$\rho u \frac{dC_i}{dx} + \frac{d}{dx}(\rho C_i U_i) = \dot{\omega}_i \tag{87}$$

where

$\dot{\omega}_i$ = rate of production of i^{th} species

C_i = mass fraction of i^{th} species

u = mean flow velocity

U_i = diffusion velocity of the i^{th} species

$u_i = u + U_i$

$\sum_i c_i = 1$

$\sum_i \rho c_i U_i = 0$

The species continuity equation does not have a simple first integral due to the fact that ρ_i is a complicated function of the flow variables.

Momentum Equation

The momentum equation is

$$\rho u \frac{du}{dx} = -\frac{dp}{dx} + \frac{d}{dx}\left[\left(\frac{4}{3}\mu + k\right)\frac{du}{dx}\right] \tag{88}$$

which has the first integral

$$\frac{\rho u^2}{2} + p - \left(\frac{4}{3}\mu + k\right)\frac{du}{dx} = \frac{\rho_o u_o^2}{2} + p_o = P \tag{89}$$

Energy Equation

The energy equation is

$$\rho u \frac{d}{dx}\left(h + \frac{u^2}{2}\right) = \left(\frac{4}{3}\mu + k\right)\frac{dy}{dx}\frac{du}{dx} - \frac{d}{dx}\left[q_x + \sum_i \rho_i h_i U_i\right] \tag{90}$$

which has the first integral

$$\rho u\left(h + \frac{u^2}{2}\right) - \left(\frac{4}{3}\mu + k\right) u \frac{du}{dx} + q_x + \sum_i \rho_i h_i U_i = \rho_o u_o\left(h_o + \frac{u_o^2}{2}\right) = \frac{Q}{2} \tag{91}$$

The quantity, q_x, for a binary mixture of molecules and atoms may be written as (Reference 20)

$$q_x = -\lambda \frac{dT}{dx} + p\,(u_a - u_m)\,\frac{D a^T \rho a U a}{\rho D_{am} C_a C_m}\left(\frac{\bar{M}}{M_m - M_a}\right)$$

$$= \text{Fourier heating} + \text{Dufour effect}$$

where

D_a^T = thermal diffusion coefficient

D_{am} = binary diffusion coefficient

$\overline{M} = M_m M_a/(C_m M_m + C_a M_a)$

λ = thermal conductivity

but,

$$u_a - u_m = (u + U_a) - (u + U_m) = U_a - U_m$$

and

$$\sum_i \rho_i U_i = 0$$

thus

$$\rho_a U_a (U_a - U_m) = - \rho U_a U_m$$

and the Dufour effect is seen to be of the order $U_a U_m$. Stated otherwise, the Dufour effect is proportional to the square of the diffusion velocity and may be neglected. The energy equation becomes

$$\rho u \left(h + \frac{u^2}{2}\right) - \left(\frac{4}{3}\mu + k\right) u \frac{du}{dx} - \lambda \frac{dT}{dx} + \sum_i \rho_i h_i U_i = \rho_o u_o \left(h_o + \frac{u_o^2}{2}\right) = \frac{Q}{2} \quad (92)$$

Upstream and downstream of the shock all the gradients, dT/dx, dv/dx and dCa/dx, just vanish and the boundary conditions may be evaluated in terms of the integration constants

$$m = \rho_o u_o$$

$$P = \frac{\rho_o u_o^2}{2} + p_o$$

$$\frac{Q}{2} = \rho_o u_o \left(h_o + \frac{u_o^2}{2}\right)$$

from equations (86) through (89), and equation (92), respectively. The conditions at the upstream end point, $x = -\infty$, will be denoted by the subscript $(\ )_{01}$, and the downstream positions, $x = +\infty$, by the subscript $(\ )_{02}$.

Thermal Equation of State

For the thermal equation of state, using Dalton's Law of partial pressures, the total pressure of a mixture of different species can be expressed as

$$\underline{P} = \sum_i p_i$$

where

$$p_i = \frac{\rho_i}{m_i} KT = n_i KT \tag{93}$$

For the case of a pure diatomic gas, equation (93) becomes

$$P = (1 + Ca)\ \rho \frac{K}{M_m}\ T = (1 + Ca)\, \rho R_m T \tag{94}$$

where

$$R_m = \frac{K}{M_m}$$

Caloric Equation of State

The caloric equation of state may be an equation for the internal energy, the enthalpy, or the specific heat. The enthalpy of the i^{th} species is given by (Reference 2)

$$h_i = \left(e_i - e_i^o\right) + \frac{p_i}{\rho_i} \tag{95}$$

where e_i is the specific internal energy for the i^{th} species

$$e_i = (e_i)_{translation} + (e_i)_{rotation} + (e_i)_{vibration}$$

$$e_i = e_i^t + e_i^r + e_i^v \tag{96}$$

The quantity, e_i^o, is the heat of formation of the i^{th} species and p_i/ρ_i is given by the thermal equation of state. The equilibrium values for e_i^t, e_i^r, and e_i^v are derived from statistical thermodynamical considerations (Reference 3)

$$e_i^t = \frac{3}{2} R_i T$$

$$e_i^r = R_i T \tag{97}$$

$$e_i^v = \left[\frac{\frac{h^* v}{kT}}{\left(e^{\frac{h^* v}{kT}} - 1\right)} \right] R_i T$$

where

h^* = Planck's constant

For the case of an ideal diatomic gas, the atoms and molecules both have an average translational energy, $3/2\ R_i T$, but molecules have, in addition, an average rotational energy, $R_i T$, and vibrational energy which varies from zero to $1/2\ R_i T$. Therefore, from equations (95), (96), and (97), we obtain:

$$h_a = \frac{5}{2} R_a T + D_m$$

$$h_m = \frac{1}{2} R_m T + e_m^v \tag{98}$$

where

$$e_a^o = -D_m$$

$$e_m^o = 0$$

but, for a diatomic gas,

$$R_a = 2R_m$$

resulting in

$$h_a = 5R_m + D_m$$

$$h_m = k_m R_m T \qquad (99)$$

where (k_m) is a function of temperature ranging between no vibrational excitation 7/2 and completely excited 9/2 (Reference 4). The specific enthalpy for the mixture may be written

$$h = \sum_i C_i h_i = C_a h_a + C_m h_m \qquad (100)$$

Using the relation $\sum_i C_i = C_a + C_m = 1$ and h_a, and h_m given by equations (99),

$$h = C_a \left[5R_m T + D_m\right] + (1 - C_a)\, k_m R_m T$$

$$h = \left[k_m + (5 - k_m)\, C_a\right] R_m T + C_a D_m \qquad (101)$$

Based upon the preceding thermodynamic considerations and the equation of change, the transition properties of the entropy function can be evaluated for chemically inert and chemically reacting flows.

ENTROPY TRANSITION PROPERTIES

The specific entropy of the mixture is given by

$$TdS = de + p\, d\left(\frac{1}{\rho}\right) \tag{102}$$

where

$$e = 3\,R_m T + C_a D_m \tag{103}$$

Differentiation of equation (103) yields

$$de = 3R_m dT + D_m dC_a \tag{104}$$

and equations (104) and (103) then yield

$$\frac{dS}{R_m} = 3\,\frac{dT}{T} + \left(\frac{D_m}{R_m T}\right) d\,C_a - (1 + C_a)\left(\frac{d\rho}{\rho}\right) \tag{105}$$

For the case of chemically reacting equilibrium flow relation (81) provides

$$\frac{C_a^{\;2}}{1 - C_a} = \frac{\rho_D}{\rho}\,\exp\left[-\frac{D_m}{R_m T}\right] \tag{106}$$

and

$$\frac{D_m}{R_m T} = \log\left[\frac{1 - C_a}{C_a^{\;2}}\left(\frac{\rho_D}{\rho}\right)\right] \tag{107}$$

is then obtained. Under these conditions, the entropy function in equation (105) becomes

$$\frac{dS}{R_m} = 3\frac{dT}{T} + \log\left(\frac{1-C_a}{C_a^2}\right) dC_a + \log\left(\frac{\rho_D}{\rho}\right) dC_a - (1+C_a)\frac{d\rho}{\rho} \tag{108}$$

Whence, by integration, we obtain the chemically reacting entropy equation

$$\frac{S-S_o}{R_m} = 3 \log T + C_a(1-2\log C_a) - (1-C_a)\log(1-C_a) - (1+C_a)\log\left(\frac{\rho}{\rho_D}\right) \tag{109}$$

From equation (109) the transition properties of the entropy function across the normal Mach disc of the rocket exhaust are given by

$$\frac{S_{02} - S_{01}}{R_m} = 3 \log\left(\frac{T_{02}}{T_{01}}\right) + \log \frac{(1-C_{01})^{1-C_{01}} (C_{01})^{2C_{01}}}{(1-C_{02})^{1-C_{02}} (C_{02})^{2C_{02}}} + (C_{02} - C_{01}) \left[1 + \log\left(\frac{\rho_D}{\rho_{01}}\right)\right] + (1 + C_{02}) \log\left(\frac{v_{02}}{v_{01}}\right) \tag{110}$$

Equation (110) is plotted in Figure 3 of this report for two values of the mass fraction parameter C_a.

For the case of chemically inert or frozen flows the mass fraction parameter remains invariant when transition through the Mach disc

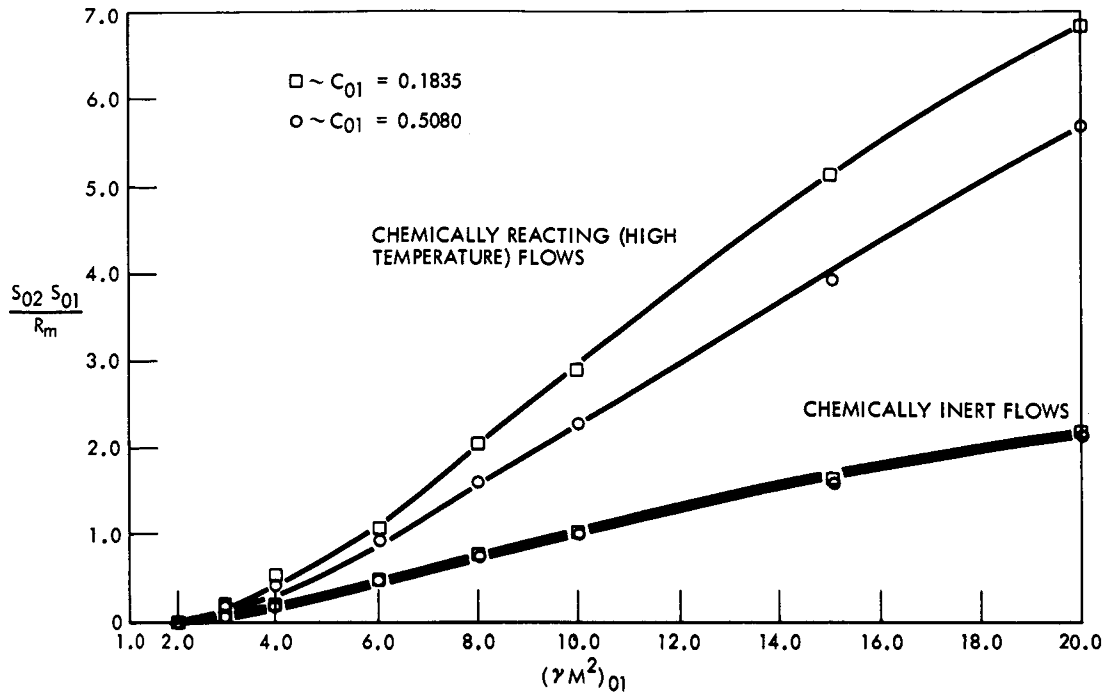

Figure 3. Entropy Production

occurs. Thus, C_{01} is identical with C_{02} and under these conditions, equation (110) results in

$$\frac{S_{02} - S_{01}}{R_m} = 3 \log\left(\frac{T_2}{T_1}\right) + (1+C_a) \log\left(\frac{v_2}{v_1}\right) \tag{111}$$

Equation (111) is plotted in Figure 3 for comparison between the two cases of chemically reacting and chemically inert flows. The plots are shown as a function of γM^2. The sample calculations were performed for the following values of the mass fraction parameter:

$$C_{01} = 0.1835$$
$$C_{01} = 0.5050 \tag{112}$$

The results of the plots indicate that, for the same initial mass fraction, the entropy increase in chemically reacting equilibrium flow is roughly double that of the chemically inert flow for lower values of the parameter γM^2. Moreover, the entropy increase for equilibrium flow is effected, to a large extent, by the mass fraction parameter whereas for frozen flow this effect is almost nil. The transition properties of the velocity ratios versus the parameter γM^2 for chemically inert and chemically reacting flows are shown in Figures 4 and 5, respectively.

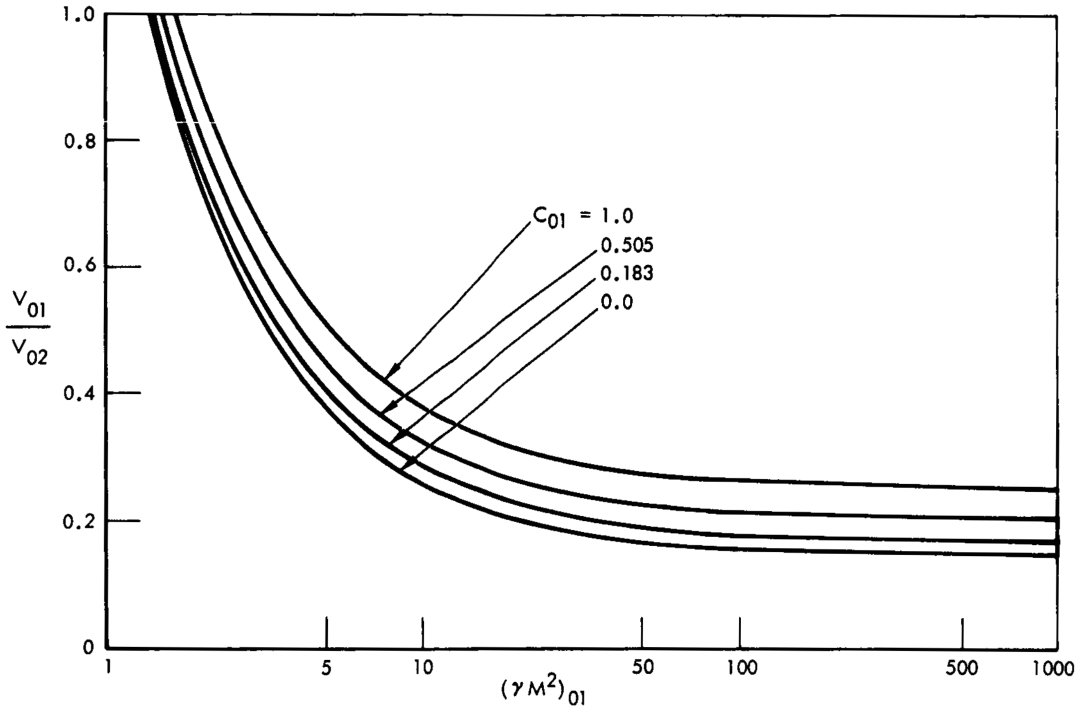

Figure 4. Velocity Ratio (V_{01}/V_{02}) for Chemically Inert Flow

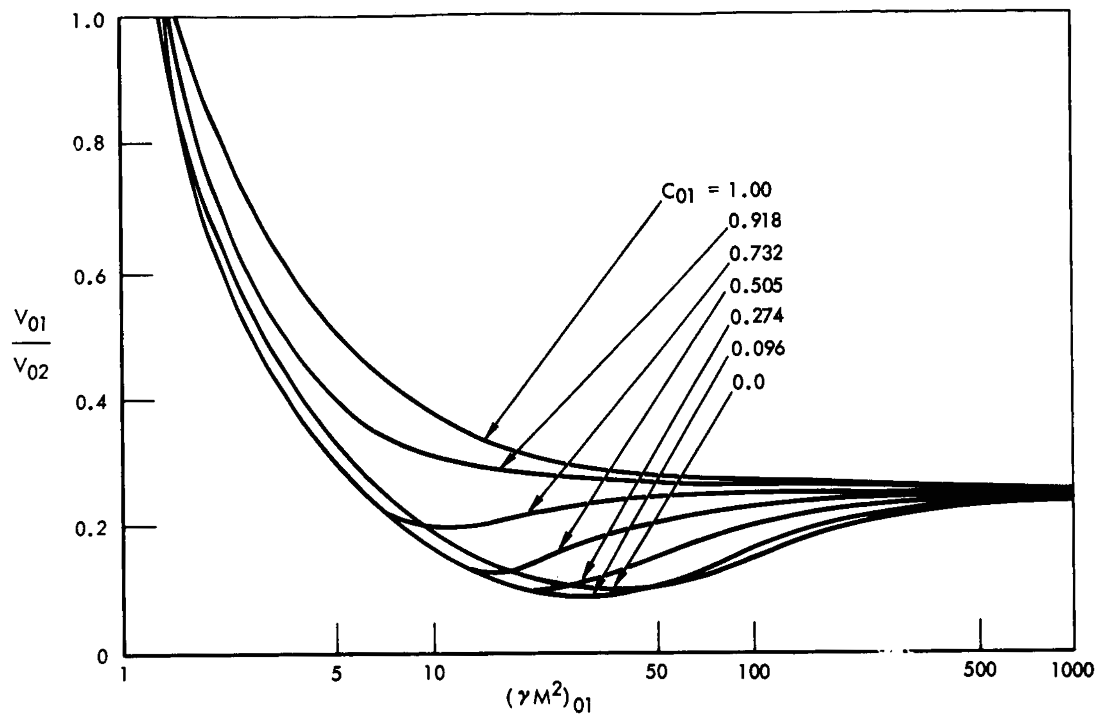

Figure 5. Velocity Ratio (V_{01}/V_{02}) for Chemically Reacting (High Temperature) Flow

V. SUMMARY AND CONCLUSIONS

The investigation of propagation characteristics of a finite amplitude acoustic pressure wave, during the phase reported here, has been concerned with the qualitative identification of the regions of predominant entropy production rates in the rocket exhaust. The derivation of the forcing function of the radiating nonlinear wave equation (Section I) in terms of the dissipating qualities of the rocket exhaust (entropy production) exhibits a close relation between the forcing function and the energy equation as well as the equation of state of the medium. Thus, within the framework of this analysis, the mechanical conditions (conservation of mass and momentum equations) are insufficient for a mathematical development of the problem at hand.

The formal derivation of the forcing function, as presented in this report, has the additional shortcoming of assuming the existence and continuity of the dependent variables up to and including second derivatives in the region considered. This restriction limits the application of the derivation, unless provisions are made to extend the formalistic meaning of the derivation to processes that exhibit highly irreversible features and discontinuous jump conditions in the regions of interest. As a matter of fact it is these irreversible features and jump conditions, appearing in the supersonic rocket exhausts, that are of greatest interest, within the framework of this analysis, by virtue of their contribution to entropy production in the flow field.

Sections II and III of this report, discuss the investigation of conditions governing the flow of the exhaust gas after transition through an oblique shock has taken place. The shape of the shock layer formed by the expanding gases emanating from the nozzle is determined by considering the reflection properties of the expansion waves upon hitting the free boundary. Their coalescence points along the boundary determine the initial shape of the shock region before the formation of the Mach disc.

Likewise, hypersonic theory considerations with initial conditions assumed to be known from oblique shock transition relations, indicate the existence of an entropy layer near the axis of symmetry in which the temperature is high, the density low, and the pressure finite.

It was also found expedient, when considering the Mach disc transition properties, to introduce chemical flow kinetics into our considerations. This was due to the appearance of dissociation phenomena in the exhaust gas, caused by the excessive temperatures of the emanating gas and the high collision rates of atoms and molecules during shock transition phenomena.

A comparison between the entropy production of chemically reacting flows to that of chemically inert flows has been attempted in Section IV.

In the addendum to this report a mathematical derivation of partial correlation principles is presented to be used as necessary in the subsequent investigations.

Within the framework of this investigation, based upon the concept of dissipative phenomena, it appears that for the case of high pressure-ratio rocket exhausts, the regions contributing most to propagation of a finite amplitude pressure wave for given initial conditions may roughly be tabulated in the sequence of their respective contributions as follows:

1. Normal shock layers (Mach discs)

2. Oblique shock layers

3. Viscous shear layers and vortex regions.

From consideration of the contributions of the normal shock layer, it appears that chemical reactions in the shock layer itself, taking place due to partially dissociated hot exhaust gas, are of primary importance; even for low Mach numbers and a small fraction of dissociated mass the entropy production increases significantly. Computations (Figure 5) indicate that the entropy production in the transition region is more than doubled as soon as critical pressure ratios are reached. This would tend to indicate that, barring the contribution of other terms in the forcing function (temperature-density product), the acoustic intensity of a hot exhaust should be at least three decibels higher than that of a cold exhaust, the increase being approximately uniform within the range of the parameter (γM^2) shown in Figure 5.

It also appears that the entropy gain of the particles, attained during transition phenomena, persists and is carried into the flow field by the streamlines, causing a high entropy gain of the fluid (as the axis of the rocket exhaust is approached) behind the first shock layer formation (Sections II and III). This indicates that in the case where chemical equilibrium is not attained in the transition phase, the nonequilibrium values will "freeze" on the streamlines and the adjustment to equilibrium flow will take place by a sudden irreversible release of the dissociation energy with a large increase of entropy, and a Mach number decrease in the successive transition layer.

The overall aspects of these phenomena will have to undergo individual analysis for quantitative results and analytical predictions.

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ADDENDUM: PARTIAL CORRELATIONS AND RESIDUAL VARIANCES

The appearance of a nonlinear forcing function in the aerodynamic noise problem formulation results in a general treatment of the solution by means of statistical correlation principles. (See Bibliography.) In the present formulation, an attempt is being made to obtain as much pertinent information as possible from extraneous sources and from the physical aspects of the problem which conform to the present approach. Certain aspects of uncoupling multiple correlation coefficients, however, serve to generate mean statistical products which are mutually independent and thus cause removal of variations due to higher order random variables.[1] These aspects are considered in the following development: since any random physical variable is suitable for application to the following formulation, the random velocity function used here can be regarded as a representative quantity; its use does not contradict the generalization of the procedure to other random variables.

Two- and three-dimensional random velocity fields are considered in this derivation and are generalized to any number of dimensions. The concept of two-dimensional partial correlations is trivial, except for exceptional cases, but it will be treated here because of its importance in the general theory.

THE TWO-DIMENSIONAL RESIDUAL VARIANCE

Let u_i $(i = 1, 2)$ represent two random velocity components so that:

$$u_1 = u_1(\underline{x}_1, t_1); \quad u_2 = u_2(\underline{x}_2, t_2) \qquad \text{(A. 1)}$$

where $[\underline{x}_1, t_1]$ and $[\underline{x}_2, t_2]$ are any points distinct from one another in the three dimensional space-time field. Under these conditions the three second-order expectations of the random variables u_1 and u_2 are given by the integrals

$$E\left(u_1^2\right) = \int du_1 \int du_2 \left(u_1^2\right) f(u_1, u_2)$$

$$E(u_1 u_2) = \int du_1 \int du_2 (u_1 u_2) f(u_1, u_2) \qquad \text{(A. 2)}$$

$$E\left(u_2^2\right) = \int du_1 \int du_2 \left(u_2^2\right) f(u_1, u_2)$$

[1]Cramer, H. Mathematical Methods of Statistics. Princeton University Press (1961).
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where $f(u_1, u_2)$ is the distribution frequency function of the two random variables u_1 and u_2.

If the means, m_1 and m_2, are assumed to be zero, then relations A.2 represent the quantities which define the correlation coefficient ρ_{12} between the two variables, which may be written

$$\rho_{12} = \frac{E(u_1 u_2)}{\sqrt{E\left(u_1^2\right)}\ \sqrt{E(u_2)^2}} \tag{A.3}$$

However, if the means, m_1 and m_2, are different from zero, relation A.3 does not hold true since the independence of the two variables u_1 and u_2 will not cause ρ_{12} to vanish—a fact upon which the concept of the correlation is based.

Next, consider the straight line in the u_1 and u_2 planes.

$$u_1^* = \beta_{12} u_2 + \alpha \tag{A.4}$$

where β_{12} and α are constant parameters and the subscripts of β_{ij} denotes that i = 1 is the independent variable and j = 2 is the variable to which the coefficient β_{ij} is attached.

Now form the difference

$$u_1 - u_1^* = u_1 - \beta_{12} u_2 - \alpha \tag{A.5}$$

which is the difference along the u_1 direction of a particle of mass $d\rho$ at (u_1, u_2) and the straight line A.4.

To find the best estimate of the random variable u_1 in terms of the line A.4, consider the mean square regression:

$$E\left\{\left(u_1 - u_1^*\right)^2\right\} = E\left\{\left(u_1 - \beta_{12} u_2 - \alpha\right)^2\right. \tag{A.6}$$

It is convenient at this point to introduce the mean variables $\overline{u}_1$ and $\overline{u}_2$, assumed constant, and write relation A.6 in the form

$$E\left\{\left(u_1 - u_1^*\right)^2\right\} = E\left\{(u_1 - \overline{u}_1) - \beta_{12}(u_2 - \overline{u}_2) + (\overline{u}_1 - \beta_{12}\overline{u}_2 - \alpha)\right\}^2 \qquad \text{(A.7)}$$

Upon expansion, relation A.7 becomes

$$E\left\{\left(u_1 - u_1^*\right)\right\} = E\left\{(u_1 - \overline{u}_1)^2\right\} + \beta_{12}^2 E\left\{(u_2 - \overline{u}_2)^2\right\} + (\overline{u}_1 - \beta_{12}\overline{u}_2 - \alpha)^2 E(1)$$

$$- 2\beta_{12} E\left\{(u_1 - \overline{u}_1)(u_2 - \overline{u}_2)\right\} + 2(\overline{u}_1 - \beta_{12}\overline{u}_2 - \alpha) E\left\{\overline{u}_1 - \overline{u}_1\right\}$$

$$- 2(\overline{u}_1 - \beta_{12}\overline{u}_2 - \alpha)\beta_{12} E\left\{u_2 - \overline{u}_2\right\} \qquad \text{(A.8)}$$

Again denoting the mean moments of the distribution by λ_i and λ_{ij} $(i = 1, 2) : (j = 1, 2)$ for first and second moments respectively and noting that, by definition of the mean, all moments $\lambda_i = 0$ $(i - 1, 2)$, relation A.8 may be written

$$E\left\{\left(u_1 - u_1^*\right)^2\right\} = \lambda_{11} + \beta_{12}^2 \lambda_{22} - 2\beta_{12}\lambda_{12} + (\overline{u}_1 - \beta_{12}\overline{u}_2 - \alpha)^2 \qquad \text{(A.9)}$$

where the last expression is a consequence of the fact that $E(1) = 1$.

In order to find the coefficients β_{12} and α which will make the expression in A.9 a minimum, the variational principles will be applied. Here, however, both α and β are parameters which do not depend upon their derivatives. Hence, the variational operator δ becomes simply the differential operation itself. Thus by differentiating with respect to the two parameters involved, the following expressions are obtained:

$$\begin{aligned} 2\beta_{12}\lambda_{22} - 2\lambda_{12} - 2(\overline{u}_1 - \beta_{12}\overline{u}_2 - \alpha)\,\overline{u}_2 &= 0 \\ 2(\overline{u}_1 - \beta_{12}\overline{u}_2 - \alpha)(-1) &= 0 \end{aligned} \qquad \text{(A.10)}$$

From the second equation,

$$(\overline{u}_1 - \beta_{12}\overline{u}_2 - \alpha) = 0 \qquad \text{(A.11)}$$

and so the first equation in A.10 becomes:

$$\beta_{12}\lambda_{22} - \lambda_{12} = 0 \tag{A.12}$$

from which it may be inferred that

$$\beta_{12} = \frac{\lambda_{12}}{\lambda_{22}} \tag{A.13}$$

Relation A.13 represents the value of the coefficient β which will make the mean square in A.9 a minimum.

For future generalization, the derived expression will be considered in a more concrete form. For this purpose, the second-order-moment matrix M given by

$$M = \begin{pmatrix} \lambda_{11} & \lambda_{12} \\ \lambda_{21} & \lambda_{22} \end{pmatrix} \tag{A.14}$$

is introduced.

Now if the determinant of this matrix is denoted by the symbol Λ and the cofactor of λ_{ij} by Λ_{ij}, then

$$\begin{aligned} \Lambda &= \epsilon_{ij}\,\lambda_{1i}\,\lambda_{2j} \\ \Lambda_{ij} &= \epsilon_{ik}\,\epsilon_{j}\,\lambda_{ke} \end{aligned} \tag{A.15}$$

Note that relation A.13 may be written

$$\beta_{12} = \frac{\lambda_{12}}{\lambda_{22}} = -\frac{\Lambda_{21}}{\Lambda_{11}} = -\frac{\epsilon_{2i}\,\epsilon_{1j}\,\lambda_{ij}}{\epsilon_{1i}\,\epsilon_{1j}\,\lambda_{ij}} \tag{A.16}$$

Moreover, because of symmetry, $\lambda_{12} = \lambda_{21}$, the preceding equation may be written in the form

$$\beta_{12} = \frac{\lambda_{21}}{\lambda_{22}} = -\frac{\Lambda_{12}}{\Lambda_{22}} = -\frac{\epsilon_{1i}\,\epsilon_{2j}\,\lambda_{ij}}{\epsilon_{1i}\,\epsilon_{1j}\,\lambda_{ij}} \tag{A.17}$$

The notation in A.17 will be used as the more symmetric one since it can be generalized to the form

$$\beta_{ij} = -\frac{\Lambda_{ij}}{\Lambda_{ii}} = -\frac{\epsilon_{ik}\,\epsilon_{j\ell}\,\lambda_{k\ell}}{\epsilon_{ik}\,\epsilon_{i\ell}\,\lambda_{k\ell}} \tag{A.18}$$

The above relations will also be expressed in terms of the correlation coefficient of the two variables u_1 and u_2. By definition of the correlation coefficient,

$$\rho_{12} = \frac{\lambda_{12}}{\sqrt{\lambda_{11}}\,\sqrt{\lambda_{22}}} = \frac{\lambda_{12}}{\sigma_1\,\sigma_2} \tag{A.19}$$

where the terms σ_i are the variances of the respective random variables; hence

$$\lambda_{12} = \rho_{12}\sigma_1\sigma_2;\ \lambda_{11} = \sigma_1^2;\ \lambda_{22} = \sigma_2^2 \tag{A.20}$$

Relation A.17 may also be written

$$\beta_{12} = -\sigma_1\,\sigma_2\,\frac{\rho_{12}}{\sigma_2\,\sigma_2} = -\frac{\sigma_1}{\sigma_2}\,\rho_{12} \tag{A.21}$$

Introducing the determinant

$$P = \begin{vmatrix} \rho_{11} & \rho_{22} \\ \rho_{21} & \rho_{22} \end{vmatrix} = \begin{vmatrix} 1 & \rho_{12} \\ \rho_{21} & 1 \end{vmatrix} = \epsilon_{ij}\,\rho_{1i}\,\rho_{2j} \tag{A.22}$$

and the cofactors

$$\rho_{ij} = \epsilon_{ik}\,\epsilon_{j\ell}\,\rho_{k\ell} \tag{A.23}$$

gives

$$\beta_{12} = - \frac{\sigma_1}{\sigma_2} \frac{P_{12}}{P_{11}} \tag{A.24}$$

Generalizing the subscripts yields

$$\beta_{ij} = - \frac{\sigma_i}{\sigma_j} \frac{P_{ij}}{P_{ii}} \tag{A.25}$$

It should be noted that the summation convention will be implied only in connection with the tensozial notation, e. g., $\epsilon_{ijk} \lambda_{jk}$, etc., and not with the expressions for determinants and cofactors.

Thus, in at least two dimensions the mean variance of the expression

$$E\left\{\left(u_1 - u_1^*\right)^2\right\} = E\left\{(u_1 - \beta_{12}u_2 - \alpha)^2\right\} \tag{A.26}$$

takes on its minimum value when the coefficient β_{12} becomes

$$\beta_{12} = - \frac{\Lambda_{12}}{\Lambda_{11}} = - \frac{\sigma_1}{\sigma_2} \frac{P_{12}}{P_{11}} \tag{A.27}$$

or generally

$$\beta_{12} = - \frac{\Lambda_{ij}}{\Lambda_{ii}} = - \frac{\sigma_i}{\sigma_j} \frac{P_{ij}}{P_{ii}} \tag{A.27}$$

Referring to relation A.9 where it was shown that

$$E\left|u_1 - u_1^*\right|^2 = \lambda_{11} + \beta_{12}^2\lambda_{22} - 2\beta_{12}\lambda_{12} + (\overline{u}_1 - \beta_{12}\overline{u}_2 - \alpha)^2 \tag{A.28}$$

Moreover, for a minimum mean square

$$\beta_{12} = - \frac{\Lambda_{12}}{\Lambda_{11}} = - \frac{\sigma_1}{\sigma_2} \frac{P_{12}}{P_{11}}; \; (\overline{u} - \beta_{12}\overline{u}_2 - \alpha) = 0 \tag{A.29}$$

Hence relation A.28 becomes

$$E\left\{\left(u_1 - u_1^*\right)^2_{min}\right\} = \lambda_{11} + \frac{\Lambda_{12}^2}{\Lambda_{11}^2}\lambda_{22} + 2\frac{\Lambda_{12}}{\Lambda_{11}}\lambda_{12} \tag{A.30}$$

which yields

$$E\left\{\left(u_1 - u_1^*\right)^2_{min}\right\} = \lambda_{11} + \frac{\lambda_{12}^2}{\lambda_{22}^2}\lambda_{22} = 2\frac{\lambda_{12}}{\lambda_{22}}\lambda_{12}$$

$$= \lambda_{11} + \frac{\lambda_{12}^2}{\lambda_{22}} - 2\frac{\lambda_{12}^2}{\lambda_{22}}$$

$$= \lambda_{11} - \frac{\lambda_{12}^2}{\lambda_{22}} \tag{A.30A}$$

$$E\left\{\left(u_1 - u_1^*\right)^2_{min}\right\} = \frac{\lambda_{11}\lambda_{22} - \lambda_{12}}{\lambda_{22}} = \frac{\Lambda}{\Lambda_{11}} = \frac{\epsilon_{ij}\lambda_{1i}\lambda_{2j}}{\epsilon_{1j}\epsilon_{1j}\lambda_{ij}} \tag{A.31}$$

Moreover, in terms of the correlation matrix,

$$\Lambda = \begin{vmatrix} \lambda_{11} & \lambda_{12} \\ \lambda_{21} & \lambda_{22} \end{vmatrix} = \begin{vmatrix} \rho_{11}\sigma_1^2 & \rho_{12}\sigma_1\sigma_2 \\ \rho_{21}\sigma_2\sigma_2 & \rho_{22}\sigma_2^2 \end{vmatrix} = \begin{vmatrix} \sigma_1^2 & \rho_{12}\sigma_1\sigma_2 \\ \rho_{21}\sigma_1\sigma_2 & \sigma_2^2 \end{vmatrix} = \sigma_1^2 \begin{vmatrix} \sigma_1 & \rho_{12}\sigma_2 \\ \rho_{21}\sigma_2 & \frac{\sigma_2^2}{\sigma_1} \end{vmatrix}$$

or, in terms of A.30A,

$$E\left(u_1 - u_1^*\right)^2 = \rho_{11}\sigma_1^2 - \frac{\rho_{12}^2\sigma_1^2\sigma_2^2}{\sigma_2^2} = \sigma_1^2\left|\rho_{11} - \rho_{12}^2\right| = \sigma_1^2\frac{P}{P_{11}} = \sigma^2 P \tag{A.32}$$

since $P_{11} = \rho_{22} = 1$.

Hence

$$E\left\{\left(u_1 - u_2^*\right)^2\right\} = \frac{\Lambda}{\Lambda_{11}} = \sigma_1^2 \frac{P}{P_{11}};$$

$$\beta_{ij} = -\frac{\Lambda_{ij}}{\Lambda_{ij}} = -\frac{\sigma_i}{\sigma_j}\frac{P_{ij}}{P_{ii}} \qquad \text{(A.33)}$$

In terms of the correlation coefficient $\rho_{12} = \rho_{21}$, relation A.33 becomes

$$E\left\{\left(u_1 - u_1^*\right)^2\right\} = \sigma_1^2\left(1 - \rho_{12}^2\right) \qquad \text{(A.34)}$$

Hence, when $\rho_{12} = \pm 1$, it is when the variables are perfectly correlated that the mean square variance of the above expression vanishes. On the other hand, when the two variables are independent, $\rho_{12} = 0$ and the mean variance is the total variance of the variable u_1.

Consider now the line of best fit given in accordance with previous assumptions by

$$u_1^* = \beta_{12}u_2 + \alpha; \qquad \text{(A.35)}$$

from relations A.11 and A.17

$$\alpha = u_1 - \beta_{12}\overline{u}_2;$$

$$\beta_{12} = -\frac{\Lambda_{12}}{\Lambda_{11}} = -\frac{\sigma_1}{\sigma_2}\frac{P_{12}}{P_{11}} \qquad \text{(A.36)}$$

where the terms $\overline{u}_i$, $i = 1, 2$ are the mean velocities.

Hence relation A.35 may be written

$$u_1^* = -\frac{\Lambda_{12}}{\Lambda_{11}} u_2 + \overline{u}_1 + \frac{\Lambda_{12}}{\Lambda_{11}} \overline{u}_2 = \overline{u}_1 - \frac{\Lambda_{12}}{\Lambda_{11}} (u_2 - \overline{u}_2)$$

or alternately

$$u_1^* - \overline{u}_1 = - \frac{\Lambda_{12}}{\Lambda_{11}} (u_2 - \overline{u}_2) = - \frac{\sigma_1}{\sigma_2} \frac{P_{12}}{P_{11}} (u_2 - \overline{u}_2) \qquad \text{(A.37)}$$

Generalizing the preceding derivation,

$$u_i^* - \overline{u}_i = - \frac{\sigma_i}{\sigma_j} \frac{P_{ij}}{P_{ii}} (u_j - \overline{u}_j) \qquad \text{(A.38)}$$

Specifically considering the line of best fit of u_2 with respect to u_1, it can be deduced from relation A.38 that

$$u_2^* - \overline{u}_2 = - \frac{\sigma_2}{\sigma_1} \frac{P_{21}}{P_{22}} (u_1 - \overline{u}_1) \qquad \text{(A.39)}$$

Hence the two possible combinations in two dimensions are given by

$$u_1^* - \overline{u}_1 = - \frac{\sigma_1}{\sigma_2} \frac{P_{12}}{P_{11}} (u_2 - \overline{u}_2);$$

$$u_2^* - \overline{u}_2 = - \frac{\sigma_2}{\sigma_1} \frac{P_{21}}{P_{22}} (u_1 - \overline{u}_1) \qquad \text{(A.40)}$$

Noting that in the case $P_{11} = P_{22} = 1$ and $P_{12} = P_{21} = \rho_{12}$, then

$$u_1^* - \overline{u}_1 = + \frac{\sigma_1}{\sigma_2} \rho_{12} (u_2 - \overline{u}_2)$$

$$\left(u_2^* - \overline{u}_2\right) = + \frac{\sigma_2}{\sigma_1} \rho_{12} (u_1 - \overline{u}_1) \qquad \text{(A.41)}$$

Hence the equations for the two regression lines of best fit are

$$\frac{u_1^* - \overline{u}_1}{\sigma_1} = \rho_{12} \frac{u_2 - \overline{u}_2}{\sigma_2}$$

$$\frac{u_1 - \overline{u}_1}{\sigma_1} = \frac{1}{\rho_{12}} \frac{u_2^* - \overline{u}_2}{\sigma_2} \qquad (A.42)$$

Both lines pass through the center of gravity or the mean velocity point $(\overline{u}_1; \overline{u}_2)$. They can never coincide unless $\rho = \pm 1$.

When $\rho = \pm 1$, the whole mass of the distribution is situated on a straight line given by any one of relations A.42. On the other hand, when $\rho = 0$,

$$u_1^* = \overline{u}_1; \; u_2^* = \overline{u}_2 \qquad (A.43)$$

and the lines become parallel to the axes and pass through the center of gravity.

It will now be shown that the residual variance is completely uncorrelated with any of the subtracted variables. Consider the quantity

$$E\left| u_2(u_1 - \beta_{12}u_2 - \alpha)\right| \qquad (A.44)$$

Since the variable u_2 is subtracted from the variable u_1 the expectation of $(u_1 - \beta_{12} - \alpha)$ is given by A.44 and it should be zero if no correlation exists.

Put relation A.44 in the form

$$E\left| u_2(u_1 - \beta_{12}u_2 - \alpha)\right| = E\left|(u_2 - \overline{u}_2)\left[(u_1 - \overline{u}_1) - \beta_{12}(u_2 - \overline{u}_2)\right.\right.$$

$$\left.+ (u_1 - \beta_{12}u_2 - \alpha)\right] + \overline{u}_2\left[(u_1 - \overline{u}_1)\right.$$

$$\left.- \beta_{12}(u_2 - \overline{u}_2) + (u_2 - \beta_{12}u_2 - \alpha)\right]$$

This obviously becomes

$$E\left\{u_2(u_1 - \beta_{12}u_2 - \alpha)\right\} = E(u_2 - \overline{u}_2)(u_1 - \overline{u}_1) - \beta_{12}E\left\{(u_2 - \overline{u}_2)^2\right.$$

$$+ (\overline{u}_1\ \beta_{12}\overline{u}_2 - \alpha)E(u_2 - \overline{u}_2)$$

$$+ \overline{u}_2 E(u_1 - \overline{u}_1) - \beta_{12}u_2 E(u_2 - \overline{u}_2)$$

$$+ \overline{u}_2(\overline{u}_1 - \beta_{12}\overline{u}_2 - \alpha)E(1)$$

and since all first order means must vanish and E (1) = 1, then

$$E\left\{u_2(u_1 - \beta_{12}u_2 - \alpha)\right\} = E\left[(u_2 - \overline{u}_2)(u_1 - \overline{u}_1)\right] - \beta_{12}E\left\{(u_2 - \overline{u}_2)^2\right\}$$

$$+ \overline{u}_2(\overline{u}_1 - \beta_{12}u_2 - \alpha) \qquad \text{(A.45)}$$

Now for minimum value, the previously derived relations are introduced:

$$(\overline{u}_1 - \beta_{12}\overline{u}_2 - \alpha) = 0;\ \beta_{12} = -\frac{\Lambda_{12}}{\Lambda_{11}} \qquad \text{(A.46)}$$

Hence relation A.45 may be written

$$E\left\{u_2(u_1 - \beta_{12}u_2 - \alpha)\right\}_{min} = E\left[(u_1 - \overline{u}_1)(u_2 - \overline{u}_2)\right] - \beta_{12}E\left[(u_2 - \overline{u}_2)^2\right]$$

$$= \lambda_{12} - \beta_{12}\lambda_{22} = \lambda_{12} + \frac{\Lambda_{12}}{\Lambda_{11}}\lambda_{22}$$

$$= \lambda_{12} - \frac{\lambda_{21}}{\lambda_{22}}\lambda_{22} = \lambda_{12} - \lambda_{21}$$

$$= \lambda_{12} - \lambda_{12} \equiv 0 \qquad \text{(A.47)}$$

Hence it is inferred that the residual variance of A.45 vanishes identically. From the preceding derivation, in accordance with A.47, it is also inferred that

$$E\left\{u_2(u_1 - \beta_{12}u_2 - \alpha)\right\}_{min} = E\left[(u_1 - \overline{u}_1)(u_2 - \overline{u}_2)\right] - \beta_{12} E\left[(u_2 - \overline{u}_2)^2\right]$$

$$= E\left\{(u_2 - \overline{u}_2)\left[(u_1 - \overline{u}_1) - \beta_{12}(u_2 - \overline{u}_2)\right]\right\}$$

(A.48)

Hence in all future generalizations the constant α can be dispensed with and by referring all variables u_i to their mean the line, plane or hyperplane of the closest fit can be generated by the relation

$$u_k - \sum_{\ell=1}^{n} \beta_{k\ell} u_\ell; \tag{A.49}$$

with $\ell \neq k$.

The preceding considerations immediately stipulate that

$$E\left\{u_2(u_1 - \beta_{12}u_2)\right\}_{min} = E\left\{(u_2 - \beta_{12}u_2)(u_1 - \beta_{12}u2)\right\} = E\left\{(u_1 - \beta_{12}u_2)^2\right\}$$

(A.50)

where it has been assumed that the variables u_i ($i = 1, 2$) are referred to their means $\overline{u}_i$ respectively.

Thus

$$E\left\{u_1 - \beta_{12}u_2 - \alpha)\right\}^2_{min} = E\left\{(u_1 - \overline{u}_1)\left[u_1 - \overline{u}_1 - \beta_{12}(u_2 - u_2)\right]\right\}$$

$$= E - \left\{\left[(u_1 - \overline{u}_1) - \beta_{12}(u_2 - u_2)\right]^2\right\}$$

(A.51)

Moreover the above deductions are, as has been shown, a consequence of the derived important principle that the residual variance of a random variable is completely uncorrelated with any of the subtracted variables.

THE THREE-DIMENSIONAL RESIDUAL VARIANCE

In sequence to the previously considered two-dimensional random velocity field, let u_i (i = 1, 2, 3) be three random velocity components such that

$$u_1 = u_1(\underline{x}_1, t_1); \; u_2 = u_2(\underline{x}_2, t_2); \; u_3 = u_3(\underline{x}_3, t_3) \tag{A.52}$$

Moreover, let $\overline{u}_i$ (i = 1, 2, 3) be the respective mean value of the velocity u_i and then form the difference

$$\eta_{1.23} = (u_1 - \beta_{12}u_2 - \beta_{13}u_3 - \alpha) \tag{A.53}$$

Consider the minimum expectation of the mean square

$$E\left\{u_1 - \beta_{12}u_2 - \beta_{13}u_3 - \alpha\right\}^2 = E\left[(\eta_{1.23})^2\right] \tag{A.54}$$

The complete analysis of the previous section will now be re-derived for the case of three random variables and the derivation generalized to higher order dimensions.

Thus relation A.53 may be written in the form

$$\begin{aligned} E(\eta_{1.23})^2 = {} & E\left[(u_1 - \overline{u}_1)^2\right] + \beta_{12}^2 E\left[(u_2 - \overline{u}_2)^2\right] + \beta_{13}^2 E\left[(u_3 - \overline{u}_3)^2\right] \\ & + \left[\overline{u}_1 - \beta_{12}\overline{u}_2 - \beta_{13}\overline{u}_3 - \alpha\right]^2 E(1) \\ & - 2\beta_{12} E\left[(u_1 - \overline{u}_1)(u_2 - \overline{u}_2)\right] - 2\beta_{13} E\left[(u_1 - \overline{u}_1)(u_3 - \overline{u}_3)\right] \\ & + 2\beta_{12}\beta_{13} E\left[(u_2 - \overline{u}_2)(u_3 - \overline{u}_3)\right] \end{aligned} \tag{A. 55}$$

$$+ 2(\overline{u}_1 - \beta_{12}\overline{u}_2 - \beta_{13}''\overline{u}_3 - \alpha)\left[\underbrace{E(u_1 - \overline{u}_1)}_{''0} - \underbrace{E(u_2 - \overline{u}_2)}_{''0}\beta_{12} - \beta_{13}\underbrace{E(u_3 - \overline{u}_3)}_{''0}\right]$$

Hence since all the mean expectation $E(u_i - \overline{u}_i) = 0$ by definition of the mean and E(1) = 1, the above variance can be written in the form

$$E(\eta_{1,23})^2 = \lambda_{11} + \beta_{12}^2\lambda_{22} + \beta_{13}^2\lambda_{33} - 2\beta_{12}\lambda_{12} - 2\beta_{13}\lambda_{13} + 2\beta_{12}\beta_{13}\lambda_{23} + \left[\overline{u}_1 - \beta_{12}\overline{u}_2 - \beta_{13}\overline{u}_3 - \alpha\right]^2 \quad (A.56)$$

Now in order to find the coefficients β_{ij} and α for a minimum value of the above expression, the variational principle is applied for each variable separately to get

$$2\beta_{12}\lambda_{22} + 2\beta_{13}\lambda_{23} + 2(\overline{u}_1 - \beta_{12}\overline{u}_2 - \beta_{13}\overline{u}_3 - \alpha)(-\overline{u}_2) - 2\lambda_{12} = 0$$

$$2\beta_{13}\lambda_{33} + 2\beta_{12}\lambda_{23} + 2(\overline{u}_1 - \beta_{12}\overline{u}_2 - \beta_{13}\overline{u}_3 - \alpha)(-\overline{u}_3) - 2\lambda_{13} = 0$$

$$2(\overline{u}_1 - \beta_{12}\overline{u}_2 - \beta_{13}\overline{u}_3 - \alpha)(-1) = 0$$

(A.57)

Applying the last relation to the first two yields

$$\beta_{12}\lambda_{22} + \beta_{13}\lambda_{23} = \lambda_{12}$$

$$\beta_{13}\lambda_{33} + \beta_{12}\lambda_{23} = \lambda_{13}$$

or (A.58)

$$\lambda_{22}\beta_{12} + \lambda_{23}\beta_{13} = \lambda_{12}$$

$$\lambda_{23}\beta_{12} + \lambda_{33}\beta_{13} = \lambda_{13}$$

Thus, the following is inferred:

$$\beta_{12} = \frac{\begin{vmatrix} \lambda_{12} & \lambda_{23} \\ \lambda_{13} & \lambda_{33} \end{vmatrix}}{\begin{vmatrix} \lambda_{22} & \lambda_{23} \\ \lambda_{23} & \lambda_{33} \end{vmatrix}}; \quad \beta_{13} = \frac{\begin{vmatrix} \lambda_{22} & \lambda_{12} \\ \lambda_{23} & \lambda_{13} \end{vmatrix}}{\begin{vmatrix} \lambda_{22} & \lambda_{23} \\ \lambda_{23} & \lambda_{33} \end{vmatrix}} \quad (A.59)$$

Now introduce, as before, the determinant matrix

$$\Lambda = \begin{vmatrix} \lambda_{11} & \lambda_{12} & \lambda_{13} \\ \lambda_{21} & \lambda_{22} & \lambda_{23} \\ \lambda_{31} & \lambda_{32} & \lambda_{33} \end{vmatrix} \tag{A.60}$$

and the cofactors

$$\Lambda_{ij} = \frac{1}{2} \epsilon_{ik\ell} \epsilon_{jmn} \lambda_{km} \lambda_{\ell n} \tag{A.61}$$

Under these conditions the coefficients β_{ij} are given by

$$\beta_{12} = \frac{\Lambda_{12}}{\Lambda_{11}}; \quad \beta_{13} = - \frac{\Lambda_{13}}{\Lambda_{11}} \tag{A.62}$$

or

$$\beta_{12} = - \frac{\epsilon_{1k\ell} \epsilon_{2mn} \lambda_{km} \lambda_{\ell n}}{\epsilon_{1k\ell} \epsilon_{1mn} \lambda_{km} \lambda_{\ell n}}; \quad \beta_{13} = - \frac{\epsilon_{1k\ell} \epsilon_{3mn} \lambda_{km} \lambda_{\ell n}}{\epsilon_{1k\ell} \epsilon_{1mn} \lambda_{km} \lambda_{\ell n}} \tag{A.63}$$

Moreover

$$\Lambda = \begin{vmatrix} \lambda_{11} & \lambda_{12} & \lambda_{13} \\ \lambda_{21} & \lambda_{22} & \lambda_{23} \\ \lambda_{31} & \lambda_{32} & \lambda_{33} \end{vmatrix} = \begin{vmatrix} \rho_{11} \sigma_1^2 & \rho_{12} \sigma_1 \sigma_2 & \rho_{13} \sigma_1 \sigma_3 \\ \rho_{21} \sigma_1 \sigma_2 & \rho_{22} \sigma_2^2 & \rho_{23} \sigma_2 \sigma_3 \\ \rho_{31} \sigma_1 \sigma_3 & \rho_{32} \sigma_2 \sigma_3 & \rho_{33} \sigma_3^2 \end{vmatrix} \tag{A.64}$$

Hence, if

$$P = \begin{vmatrix} \rho_{11} & \rho_{12} & \rho_{13} \\ \rho_{21} & \rho_{22} & \rho_{23} \\ \rho_{31} & \rho_{32} & \rho_{33} \end{vmatrix}$$

then, with the respective cofactors P_{ij},

$$\Lambda_{12} = \sigma_1 \sigma_2 \sigma_3^2 P_{12}; \quad \Lambda_{13} = \sigma_1 \sigma_2^2 \sigma_3 P_{13}; \quad \Lambda_{11} = \sigma_2^2 \sigma_3^2 P_{11} \tag{A.65}$$

Hence relation A.63 may also be put in terms of the correlation coefficients:

$$\beta_{12} = -\frac{\Lambda_{12}}{\Lambda 11} = -\frac{\sigma_1 \sigma_2 \sigma_3^2}{\sigma 2 \sigma 2_3} \frac{P_{12}}{P_{11}} = -\frac{\sigma_1}{\sigma 2} \frac{P_{12}}{P_{11}} \tag{A.66}$$

and also

$$\beta_{13} = -\frac{\Lambda_{13}}{11} = -\frac{\sigma_1}{\sigma 3} \frac{P_{13}}{P_{11}} \tag{A.67}$$

Hence generally irrespective of dimensions,

$$\beta_{ij} = -\frac{\Lambda_{ij}}{\Lambda_{ii}} = -\frac{\sigma_i}{\sigma_j} \frac{P_{ij}}{P_{ii}} \tag{A.68}$$

where no summation convention is used in the subscript of the cofactors.

Now consider the residual variance given by

$$E(\eta_{1.23})^2_{min} = \lambda_{11} + \beta_{12}^2 \lambda_{22} + \beta_{13}^2 \lambda_{33} - 2\beta_{12} \lambda_{12} - 2\beta_{13} \lambda_{13} + 2\beta_{12} \beta_{13} \lambda_{23} + (\bar{u}_1 - \beta_{12} \bar{u}_2 - \beta_{13} \bar{u}_3 - \alpha)^2 \tag{A.69}$$

For a minimum, it is necessary that in accordance with A.57 and A.57 and A.68,

$$E(\eta_{1.23})^2_{min} = \lambda_{11} + \beta_{12}^2 \lambda_{22} + \beta_{13}^2 \lambda_{33} - 2\beta_{12} \lambda_{12} - 2\beta_{13} \lambda_{13} + 2\beta_{12} \beta_{13} \lambda_{23} \tag{A.70}$$

with the terms β_{ij} as given in A.68.

This yields

$$E(\eta_{1.23})^2_{min} = \frac{1}{\Lambda_{11}}\Big[(\Lambda_{11}\lambda_{11} + \Lambda_{12}\lambda_{12} + \Lambda_{13}\lambda_{13})$$

$$+ \frac{1}{\Lambda_{11}}(\Lambda_{11}\Lambda_{12}\lambda_{12} + \Lambda_{11}\Lambda_{13}\lambda_{13}$$

$$+ \Lambda_{12}\Lambda_{12}\lambda_{22} + \Lambda_{13}\Lambda_{13}\lambda_{33}$$

$$+ 2\Lambda_{12}\Lambda_{13}\lambda_{23})\Big] \tag{A.71}$$

But

$$\Lambda_{11}\lambda_{11} + \Lambda_{12}\lambda_{12} + \Lambda_{13}\lambda_{13} = \Lambda_{ij}\lambda_{ij} = \frac{1}{2}\epsilon_{\rho g}\epsilon_{jrs}\lambda_{\rho r}\lambda_{gs}\lambda_{ij}$$

$$= \epsilon_{ijk}\lambda_{1i}\lambda_{2j}\lambda_{3k} \equiv \Lambda \tag{A.72}$$

Moreover,

$$\Lambda_{11}\Lambda_{12}\lambda_{12} + \Lambda_{11}\Lambda_{13}\lambda_{13} + \Lambda_{12}\Lambda_{12}\lambda_{22} + \Lambda_{13}\Lambda_{13}\lambda_{33}$$

$$+ 2\Lambda_{12}\Lambda_{13}\lambda_{23} = \Lambda_{12}\Lambda_{1j}\lambda_{j2} + \Lambda_{13}\Lambda_{1j}\lambda_{j3}$$

(Summation convention used.) This becomes:

$$\Lambda_{12}\Lambda_{1j}\lambda_{j2} + \Lambda_{13}\Lambda_{1j}\lambda_{j3} = \frac{1}{2}\Big[\Lambda_{12}\epsilon_{jrs}\lambda_{2r}\lambda_{2j}\lambda_{3s}\Big]$$

$$- \frac{1}{2}\Big[\epsilon_{jrs}\lambda_{j2}\lambda_{2s}\lambda_{3r}\Big] + \frac{1}{2}\Big[\Lambda_{13}\epsilon_{jrs}\lambda_{j3}\lambda_{2r}\lambda_{3s}\Big] \tag{A.73}$$

$$- \frac{1}{2}\Big[\epsilon_{jrs}\lambda_{3}\lambda_{3r}\lambda_{2s}\Big]$$

Noting that in all terms of the last expression the subscript 2 is repeated, a determinant expression is obtained whose two rows or two columns are identical. Hence the above terms vanish identically for all repeated subscripts, i.e., subscripts 2 and 3 in A. 73.

It follows immediately that relation A. 71 becomes

$$E\,(\eta_{1.23})^2 = \frac{\Lambda}{\Lambda_{11}}\,; \qquad \text{(A. 74)}$$

Moreover, it the residual variance is considered,

$$E\left\{(u_1-\bar{u}_1)\left[(u_1-\bar{u}_1)^2\right] - \beta_{12}(u_2-\bar{u}_2) - \beta_{13}(u_3-\bar{u}_3)\right\} =$$

$$= E\left[(u_1-\bar{u}_1)^2\right] - \beta_{12}\,E\left[(u_1-\bar{u}_1)(u_2-\bar{u}_2)\right] - \beta_{13}\left[(u_1-\bar{u}_1)(u_3-\bar{u}_3)\right] =$$

$$= \lambda_{11} - \beta_{12}\,\lambda_{12} - \beta_{13}\,\lambda_{13} \qquad \text{(A. 75)}$$

Now, using relations A. 68 in this expression yields the minimum variance:

$$E\left\{(u_1-\bar{u}_1)\left[(u_1-\bar{u}_1) - \beta_{12}(u_2-\bar{u}_2) - \beta_{13}(u_3-\bar{u}_3)\right]\right\} =$$

$$= \lambda_{11} + \frac{\Lambda_{12}\,\lambda_{12}}{\Lambda_{11}} + \frac{\Lambda_{13}}{\Lambda_{11}}\,\lambda_{13} = \frac{1}{\Lambda_{11}}\left[\Lambda_{11}\,\lambda_{11} + \Lambda_{12}\,\lambda_{12} + \Lambda_{13}\,\lambda_{13}\right]$$

$$= \frac{\Lambda}{\Lambda_{11}} \qquad \text{(A. 76)}$$

Hence it is inferred that

$$E\left[(\eta_{1.23})^2_{min}\right] = E\left\{\left[(u_1-\bar{u}_1) - \beta_{12}(u_2-\bar{u}_2) - \beta_{13}(u_3-\bar{u}_3)\right.\right.$$

$$\left. + (u_1 - \beta_{12}u_2 - \beta_{13}u_3 - \omega)\right]^2 \qquad \text{(A. 77)}$$

$$= E\left\{(u_1-\bar{u}_1)\left[(u_1-\bar{u}_1) - \beta_{12}(u_2-\bar{u}_2) - \beta_{13}(u_3-\bar{u}_3)\right]\right.$$

This shows that the subtracted variables have a vanishing variance as stipulated above. This can also be seen by considering

$$E\left[(\eta_{2.123})^2\right] = E\left[(u_2 - \bar{u}_2)(u_1 - \bar{u}_1) - \beta_{12}(u_2 - \bar{u}_2) - \beta_{13}(u_3 - \bar{u}_3)\right] =$$

$$= \frac{1}{2}\epsilon_{123}\left[\epsilon_{jrs}\lambda_{2r}\lambda_2\ \lambda_{35}\right] + \frac{1}{2}\epsilon_{132}\left[\epsilon_{jrs}\lambda_{3r}\lambda_{2s}\lambda_{2j}\right] \equiv 0 \tag{A.78}$$

due to repeated subscripts 2 and 3.

Hence, generalizing to higher dimensions we again deduce that the residual variance of any subtracted variable is uncorrelated and thus it must vanish identically.

Hence it has been shown that

$$E\left\{u_i\,\eta_{1.23\ldots}\right\} = \frac{1}{\Lambda_{11}}\sum_{k=1}^{n}\lambda_{ik}\Lambda_{1k} = \begin{cases} \dfrac{\Lambda}{\Lambda_{11}} & \text{for } i = 1 \\ 0 & \text{for } i = 2, 3, \ldots. \end{cases} \tag{A.79}$$

This relationship in terms of the correlation matrix yields

$$\Lambda = \epsilon_{ijk}\lambda_{ij}\lambda_{2j}\lambda_{3k} = (\epsilon_{ijk}\rho_{1j}\rho_{2j}\rho_{3k})\,\sigma_1\sigma_2\sigma_3\sigma_i\sigma_j\sigma_k = \tag{A.80}$$

$$= \sigma_1^2\sigma_2^2\sigma_3^2\left[\epsilon_{ijk}\rho_{1i}\rho_{2j}\rho_{3k}\right] = \sigma_1^2\sigma_2^2\sigma_3^2\ P$$

where P is the determinant of the correlation matrix ρ_{ij}.

On the other hand, consider the cofactor

$$\Lambda_{11} = \frac{1}{2}\epsilon_{1jk}\epsilon_{1m\ell}\lambda_{jm}\lambda_{k\ell} = \frac{1}{2}\epsilon_{1jk}\epsilon_{1m\ell}\rho_{jm}\rho_{k\ell}(\sigma_j\sigma_m\sigma_k\sigma_\ell) \tag{A.81}$$

Now the subscripts jm and $k\ell$ can take on two values only, 2 and 3, so that they form the following combinations ($m \neq \ell$: $j \neq k$):

$$\sigma_2^2 \; \sigma_3^2 \qquad m = 2; \quad \ell = 3; \quad j = 2; \quad k = 3;$$

$$\sigma_2^2 \; \sigma_3^2 \qquad m = 3; \quad \ell = 2; \quad j = 2; \quad k = 3;$$

$$\sigma_2^2 \; \sigma_3^2 \qquad m = 2; \quad \ell = 3; \quad j = 3; \quad k = 2; \tag{A.82}$$

$$\sigma_2^2 \; \sigma_3^2 \qquad m = 3; \quad \ell = 2; \quad j = 3; \quad k = 2;$$

Hence

$$\Lambda_{11} = \frac{1}{2} \epsilon_{1jk} \epsilon_{1dk} \epsilon_{1m\ell} \lambda_{k\ell} = \frac{1}{2} \sigma_2^2 \sigma_3^2 \left[\epsilon_{1jk} \epsilon_{1m\ell} \rho_{jm} \rho_{k\ell} \right] \tag{A.83}$$

and

$$E\left[u_1 \eta_{1.23\cdots} \right] = \frac{\sigma_1^2 \sigma_2^2 \sigma_3^2 \Lambda}{\sigma_2^2 \sigma_3^2 \Lambda_{11}} = \sigma_1^2 \frac{\Lambda}{\Lambda_{11}} = \sigma_1^2 \frac{2\epsilon_{ijk} \rho_{ij} \rho_{2j} \rho_{3k}}{\epsilon_{1jk} \epsilon_{1m\ell} \rho_{jm} \rho_{k\ell}} \tag{A.84}$$

which formulae may be generalized to n dimensions.

Now the correlation between the variables u_1 and u_2 is measured by the correlation coefficient ρ_{12} which is sometimes called the total correlation coefficient of u_1 and u_2. However if u_1 and u_2 are considered in conjunction with n-2, further variables u_3, $u_4 \ldots\ldots u_n$, the variation of the remaining variables may be examined. Consider now the residuals

$$\eta_{1.34..} = u_1 - \beta_{13} u_3 - \beta_{14} u_4 - \cdots\cdots\cdots \beta_{1n} u_n$$

$$\eta_{2.34..} = u_2 - \beta_{13} u_3 - \beta_{14} u_4 - \cdots\cdots\cdots \beta_{1n} u_n \tag{A.85}$$

In accordance with the previous derivation, these residuals represent those parts of the variables u_1 and u_2 respectively which remain after subtraction of the best linear estimates in terms of $u_3 \ldots\ldots\ldots u_n$. Hence, the correlation coefficient between these two residuals may be regarded as a measure of the correlation between u_1 and u_2 after removal of any part of the variation due to the influence of the remaining variables $u_3, u_4 \ldots\ldots u_n$. The coefficient of the residuals in A. 85 will be referred to as the partial correlation coefficient of u_1 and u_2 with respect to $u_3, u_4 \ldots\ldots u_n$, and denoted by the notation $\rho_{12.3\ldots\ldots n}$. Hence, by A. 85

$$\rho_{12.3\ldots\ldots n} = \frac{E\left\{\eta_{1.34\ldots n}\,\eta_{2.34\ldots n}\right\}}{\sqrt{E\left\{\eta^2_{1.34\ldots n}\right\} E\left\{\eta^2_{2.34\ldots n}\right\}}} \qquad \text{(A. 86)}$$

which is an ordinary correlation coefficient between two random variables A. 80. From relation A. 86 the above coefficient will be derived for the four-dimensional case and generalized immediately to the case of n-dimensions. Thus let u_1, u_2, u_3 and u_4 be four random variables. Then consider the correlation

$$\rho_{12.34} = \frac{E\left(\eta_{1.34}\,\eta_{2.34}\right)}{E\left(\eta^2_{1.34}\right) E\left(\eta^2_{2.34}\right)} \qquad \text{(A. 87)}$$

Note that

$$\begin{aligned} E(\eta_{1.34}\eta_{2.34}) &= E\left[(u_1 - \beta_{13}u_3 - \beta_{14}u_4)(u_2 - \beta_{23}u_3 - \beta_{24}u_4)\right] \\ &= \lambda_{12} - \beta_{13}\lambda_{23} - \beta_{23}\lambda_{13} - \beta_{24}\lambda_{14} - \beta_{14}\lambda_{2u} \\ &\quad + \beta_{13}\beta_{23}\lambda_{33} + \beta_{13}\beta_{24}\lambda_{34} + \beta_{14}\beta_{23}\lambda_{34} + \beta_{14}\beta_{24}\lambda_{44} \end{aligned}$$

Thus

$$E(\eta_{1.23}\eta_{2.34}) = \lambda_{12} - \beta_{13}\lambda_{23} - \beta_{14}\lambda_{24} - \beta_{23}\lambda_{13} - \beta_{24}\lambda_{14}$$

$$+ \beta_{13}\beta_{23}\lambda_{33} + \beta_{13}\beta_{24}\lambda_{34} + \beta_{14}\beta_{23}\lambda_{34} + \beta_{14}\beta_{24}\lambda_{44} \quad \text{(A. 88)}$$

Hence for a minimum it is necessary that

$$-\lambda_{23} + \beta_{23}\lambda_{33} + \beta_{24}\lambda_{34} = 0$$

$$-\lambda_{24} + \beta_{23}\lambda_{34} + \beta_{24}\lambda_{44} = 0$$

$$-\lambda_{13} + \beta_{13}\lambda_{33} + \beta_{14}\lambda_{43} = 0$$

$$-\lambda_{14} + \beta_{13}\lambda_{34} + \beta_{14}\lambda_{44} = 0 \quad \text{(A. 89)}$$

Hence

$$\beta_{23}\lambda_{33} + \beta_{24}\lambda_{34} = \lambda_{23}$$

$$\beta_{23}\lambda_{34} + \beta_{24}\lambda_{44} = \lambda_{24} \quad \text{(A. 90)}$$

$$\beta_{13}\lambda_{33} + \beta_{14}\lambda_{43} = \lambda_{13}$$

$$\beta_{13}\lambda_{34} + \beta_{14}\lambda_{44} = \lambda_{14} \quad \text{(A. 91)}$$

Solving the above for the terms β_{ij} gives

$$\beta_{23} = \frac{\begin{vmatrix} \lambda_{23} & \lambda_{43} \\ \lambda_{24} & \lambda_{44} \end{vmatrix}}{\begin{vmatrix} \lambda_{33} & \lambda_{34} \\ \lambda_{43} & \lambda_{44} \end{vmatrix}} \qquad \beta_{24} = \frac{\begin{vmatrix} \lambda_{33} & \lambda_{23} \\ \lambda_{34} & \lambda_{24} \end{vmatrix}}{\begin{vmatrix} \lambda_{33} & \lambda_{34} \\ \lambda_{43} & \lambda_{44} \end{vmatrix}} \tag{A.92}$$

$$\beta_{13} = \frac{\begin{vmatrix} \lambda_{13} & \lambda_{43} \\ \lambda_{14} & \lambda_{44} \end{vmatrix}}{\begin{vmatrix} \lambda_{33} & \lambda_{43} \\ \lambda_{34} & \lambda_{44} \end{vmatrix}} \qquad \beta_{14} = \frac{\begin{vmatrix} \lambda_{33} & \lambda_{13} \\ \lambda_{34} & \lambda_{14} \end{vmatrix}}{\begin{vmatrix} \lambda_{33} & \lambda_{43} \\ \lambda_{34} & \lambda_{44} \end{vmatrix}} \tag{A.93}$$

Now consider the matrix

$$\Lambda = \begin{vmatrix} \lambda_{11} & \lambda_{12} & \lambda_{13} & \lambda_{14} \\ \lambda_{21} & \lambda_{22} & \lambda_{23} & \lambda_{24} \\ \lambda_{31} & \lambda_{32} & \lambda_{33} & \lambda_{34} \\ \lambda_{41} & \lambda_{42} & \lambda_{43} & \lambda_{44} \end{vmatrix} \tag{A.94}$$

Thus if $\Lambda_{ij} \cdot k\ell$ denotes the cofactor determinants of the elements ij and $k\ell$ respectively, it is deduced from A.92, A.93 and A.94 that

$$\beta_{23} = -\frac{\Lambda_{11.32}}{\Lambda_{11.22}} = -\frac{\Lambda_{11.23}}{\Lambda_{11.22}}$$

$$\beta_{24} = -\frac{\Lambda_{11.24}}{\Lambda_{11.22}} \tag{A. 95}$$

(Equation A.95 cont next page)

$$\beta_{13} = - \frac{\Lambda_{22.13}}{\Lambda_{22.11}}$$

$$\beta_{14} = - \frac{\Lambda_{22.14}}{\Lambda_{11.22}} \qquad (A.95)$$

Substituting relation A.95 in A.88 gives

$$E\ (\eta_{1.34}\, \eta_{2.34}) = \Bigg[\lambda_{12} + \frac{\Lambda_{11.23}\, \lambda_{13}}{\Lambda_{11.22}} + \frac{\Lambda_{11.24}\, \lambda_{14}}{\Lambda_{11.22}} + \frac{\Lambda_{22.13}}{\Lambda_{22.11}} \lambda_{23}$$

$$+ \frac{\Lambda_{22.14}}{\Lambda_{22.11}} \lambda_{24} + \frac{\Lambda_{22.13}}{\Lambda_{22.11}} \frac{\Lambda_{11.23}}{\Lambda_{11.22}} \lambda_{33}$$

$$+ \frac{\Lambda_{22.13}}{\Lambda_{22.11}} \frac{\Lambda_{11.24}}{\Lambda_{11.22}} \lambda_{34} + \frac{\Lambda_{22.13}}{\Lambda_{22.11}} \frac{\Lambda_{11.23}}{\Lambda_{11.22}} \lambda_{33}$$

$$+ \frac{\Lambda_{22.13}}{\Lambda_{22.11}} \frac{\Lambda_{11.24}}{\Lambda_{11.22}} \lambda_{34} + \frac{\Lambda_{22.14}}{\Lambda_{22.11}} \frac{\Lambda_{11.23}}{\Lambda_{11.22}} \lambda_{43}$$

$$+ \frac{\Lambda_{22.14}}{\Lambda_{22.11}} \frac{\Lambda_{11.24}}{\Lambda_{11.22}} \lambda_{44} \Bigg] \qquad (A.96)$$

Now, noting that $\Lambda_{11.22} = \Lambda_{22.11}$, put relation A.96 in the form

$$E\ (\eta_{1.34}\, \eta_{2.34}) = \frac{1}{\Lambda_{11.22}} \Big\{ \Lambda_{11.22}\, \lambda_{12} + \Lambda_{11.23}\, \lambda_{13} + \Lambda_{11.24}\, \lambda_{14} \Big\}$$

$$+ \frac{1}{\Lambda_{11.22}} \frac{1}{\Lambda_{11.22}} \Big\{ \Lambda_{11.22}\, \Lambda_{22.13}\, \lambda_{23}$$

$$+ \Lambda_{11.22}\, \Lambda_{22.14}\, \lambda_{24} + \Lambda_{11.23}\, \Lambda_{22.13}\, \lambda_{33}$$

$$+ \Lambda_{11.24}\, \Lambda_{22.13}\, \lambda_{34} + \Lambda_{11.23}\, \Lambda_{22.14}\, \lambda_{43}$$

$$+ \Lambda_{11.24}\, \Lambda_{22.14}\, \lambda_{44} \Big\} \qquad (A.97)$$

This yields

$$\Lambda_{11.22}\lambda_{12} + \Lambda_{11.23}\lambda_{13} + \Lambda_{11.24}\lambda_{14} = \sum_{j=2}^{4}\lambda_{ij}\Lambda_{aj.11} = -\Lambda_{21} = \Lambda_{12} \quad \text{(A.98)}$$

since:

$$\sum_{j=2}\lambda_{ij}\Lambda_{2j.11} = + \begin{vmatrix} \lambda_{12} & \lambda_{13} & \lambda_{14} \\ \lambda_{32} & \lambda_{33} & \lambda_{34} \\ \lambda_{42} & \lambda_{43} & \lambda_{44} \end{vmatrix} = -\Lambda_{21} = -\Lambda_{12} \quad \text{(A.99)}$$

by reference to relation A.94. Considering also the second expression in A.97 gives

$$\Lambda_{22.13}\left|\Lambda_{11.22}\lambda_{23} + \Lambda_{11.23}\lambda_{33} + \Lambda_{11.24}\lambda_{43}\right|$$

$$+ \Lambda_{22.14}\left|\Lambda_{11.22}\lambda_{24} + \Lambda_{11.23}\lambda_{34} + \Lambda_{11.24}\lambda_{44}\right| = \quad \text{(A.100)}$$

$$\Lambda_{22.13}\sum_{j=2}^{4}\Lambda_{11.2j}\lambda_{3\partial} + \Lambda_{22.14}\sum_{j=2}\Lambda_{11.2j}\lambda_{4j} = 0$$

and both expressions vanish identically, since the subscript j is summed over 2, 3 and 4, giving

$$\Lambda_{11} = \begin{vmatrix} \lambda_{22} & \lambda_{23} & \lambda_{24} \\ \lambda_{32} & \lambda_{33} & \lambda_{34} \\ \lambda_{42} & \lambda_{43} & \lambda_{44} \end{vmatrix} \quad \Lambda_{22} = \begin{vmatrix} \lambda_{13} & \lambda_{14} & \lambda_{11} \\ \lambda_{33} & \lambda_{34} & \lambda_{31} \\ \lambda_{43} & \lambda_{44} & \lambda_{41} \end{vmatrix} \quad \text{(A.101)}$$

so that the terms λ_{22}, λ_{23}, and λ_{24} are replaced in Λ_{11} by λ_{23}, λ_{33} and λ_{34}, which is identical with λ_{32}, λ_{33} and λ_{34}, and so that the two rows in $\Lambda_{11.2j}$ λ_{3j} become identical and the determinant vanishes. Similarly for $\Lambda_{11.2j}$ λ_{4j}. Hence relation A.97 becomes

$$E\ (\eta_{1.34}\ \eta_{2.34}) = \frac{1}{\Lambda_{11.22}} \sum_{j=2} \lambda_{1j}\ \Lambda_{2j} = -\frac{\Lambda_{12}}{\Lambda_{11.22}} \qquad \text{(A.102)}$$

Consider next the expression

$$E\ \left|\eta^2_{1.34}\right| = E\ (u_1 - \beta_{13}u_3 - \beta_{14}u_4)^2 = E\left[u_1(u_1 - \beta_{13}u_3 - \beta_{14}u_4)\right]$$

$$= \lambda_{11}\quad \beta_{13}\ \lambda_{13} - \beta_{14}\ \lambda_{14} \qquad \text{(A. 103)}$$

But it is also true that

$$\beta_{13} = \frac{\Lambda_{22.13}}{\Lambda_{11.22}}$$

$$\beta_{14} = \frac{\Lambda_{22.14}}{\Lambda_{11.22}} \qquad \text{(A.104)}$$

Hence

$$E\ \left|\eta^2_{1.34}\right| = \frac{1}{\Lambda_{11.22}}\ \left[\Lambda_{11.22}\ \lambda_{11} + \Lambda_{22.13}\ \lambda_{13} + \Lambda_{22.14}\lambda_{14}\right] \qquad \text{(A.105)}$$

$$= \frac{1}{\Lambda_{11.22}}\ \left[\Lambda_{22.11}\lambda_{11} + \Lambda_{22.13}\lambda_{13} + \Lambda_{22.14}\ \lambda_{14}\right]$$

Referring to relation A.101, it is noted that the above is equivalent to substituting for λ_{11}, λ_{31} and λ_{41} the terms λ_{11}, λ_{13} and λ_{14}, which again leave Λ_{22} unchanged. Hence

$$E\ \left|\eta^2_{2.34}\right| = \frac{1}{\Lambda_{11.22}} \sum_{\substack{j=1 \\ j\neq 2}}^{4} \lambda_{ij}\ \Lambda_{22.ij} = \frac{\Lambda_{22}}{\Lambda_{11.22}} \qquad \text{(A.106)}$$

Generalizing to relation $E\ \left(\eta^2_{2.34}\right)$ gives

$$E\ \left(\eta^2_{2.34}\right) = \frac{1}{\Lambda_{11.22}} \sum_{j=2}^{4} \lambda_{2j}\ \Lambda_{2j} = \frac{\Lambda_{11}}{\Lambda_{11.22}} \qquad \text{(A.107)}$$

Hence considering the partial correlation coefficient

$$\rho_{12.34} = \frac{E(\eta_{1.34}\,\eta_{2.34})}{\sqrt{E\left(\eta^2_{1.34}\right)\,E\left(\eta^2_{2.34}\right)}} \qquad \text{(A.108)}$$

it follows from A.102, A.106 and A.107 that

$$\rho_{12.34} = -\frac{\dfrac{\Lambda_{12}}{\Lambda_{11.22}}}{\sqrt{\dfrac{\Lambda_{22}\,\Lambda_{11}}{\Lambda_{11.22}}}} = -\frac{\Lambda_{12}}{\sqrt{\Lambda_{11}\,\Lambda_{22}}} \qquad \text{(A.109)}$$

In terms of the correlation coefficients,

$$-\frac{\Lambda_{12}}{\Lambda_{11}\Lambda_{22}} = -\sigma_1\,\sigma_2\,\frac{P_{12}}{P_{11.22}}$$

$$\frac{\Lambda_{11}}{\Lambda_{11.22}} = \sigma_1^2\,\frac{P_{11}}{P_{11.22}}$$

$$\frac{\Lambda_{22}}{\Lambda_{11.22}} = \sigma_2^2\,\frac{P_{22}}{P_{11.22}}$$

Hence

$$\rho_{12.34} = -\frac{P_{12}}{P_{11}P_{22}} \qquad \text{(A.110)}$$

For the case of three dimensions, considering the matrix

$$P = \begin{vmatrix} \rho_{11} & \rho_{12} & \rho_{13} \\ \rho_{21} & \rho_{22} & \rho_{23} \\ \rho_{31} & \rho_{32} & \rho_{33} \end{vmatrix} \qquad \text{(A.111)}$$

it follows that

$$- P_{12} = \begin{vmatrix} \rho_{23} & \rho_{21} \\ \rho_{33} & \rho_{31} \end{vmatrix} = - (\rho_{23} \rho_{31} - \rho_{12}) = \rho_{12} - \rho_{13} \rho_{23} \quad \text{(A. 112)}$$

since $\rho_{33} = 1$; also

$$P_{11} = \rho_{22} \rho_{33} - \rho_{23} \rho_{32} = \left(1 - \rho_{23}^2\right)$$

$$P_{22} = \rho_{11} \rho_{33} - \rho_{13} \rho_{31} = \left(1 - \rho_{13}^2\right) \quad \text{(A. 113)}$$

Hence for the three-dimensional case the correlation coefficient becomes

$$\rho_{12.3} = \frac{\rho_{12} - \rho_{13} \rho_{23}}{\sqrt{\left(1 - \rho_{13}^2\right) \left(1 - \rho_{23}^2\right)}} \quad \text{(A. 114)}$$

and similarly for other dimensions.

It is noted that in the case of uncorrelated variables, say when $\rho_{13} = \rho_{23} = 0$, then

$$\rho_{12.3} = \rho_{12} \quad \text{(A. 115)}$$

and the partial correlation coefficient is equal to the total correlation coefficient.

Now consider briefly the definition of a multiple correlation coefficient. The residual is defined by

$$\eta_{1.23....n} = u_1 - \sum_{j=2}^{n} \beta_{ij} u_j = (u_1 - u_1^*) \quad \text{(A. 116)}$$

where

$$u_1^* = \sum_{j=2}^{n} \beta_{ij} u_j$$

Now among all linear combinations of u_i, $i = 2 . . . . . n$, it is the coefficient u_1^* which has the maximum correlation (or a minimum value) with respect to u_i.

The correlation coefficient

$$\rho_{1(23.....n)} = \frac{E\left(u_1 u_1^*\right)}{\sqrt{E\left(u_1^2\right) E\left(u_1^*\right)^2}} \qquad \text{(A. 117)}$$

is the measure of correlation between u_1 and the totality of all the remaining variables. This coefficient will be referred to as the multiple correlation coefficient between u_1 and u_i $(i = 2, 3, ... n)$.

Consider now the quantity

$$E\left(u_1 u_1^*\right) = \Big\{E\ u_1(u_1 - \eta_{1.\,23.\,n}) = E(u_1 u_1) - E(u_1 \eta_1)$$

$$= \lambda_{11} - \frac{\Lambda}{\Lambda_{11}} \qquad \text{(A. 118)}$$

by previous derivations. Also,

$$E\left(u_1^2\right) = E(u_1 u_1) = \lambda_{11}$$

$$E\left(u_1^{*2}\right) = E(u_1 u_1 - \eta_{1.\,2.\,3}) = \lambda_{11} - \frac{\Lambda}{\Lambda_{11}} \qquad \text{(A. 119)}$$

Hence

$$\rho_{1(234..n)} = \frac{\lambda_{11} - \frac{\Lambda}{\Lambda_{11}}}{\sqrt{\lambda_{11}\left[\lambda_{11} - \frac{\Lambda}{\Lambda_{11}}\right]}} = \frac{\lambda_{11}\Lambda_{11} - \Lambda}{\Lambda_{11}\sqrt{\frac{\lambda_{11}(\lambda_{11}\;{}_{11} - \Lambda)}{\Lambda_{11}}}} \qquad \text{(A. 120)}$$

This yields

$$\rho_{1(23...n)} = \frac{\lambda_{11}\Lambda_{11} - \Lambda}{\sqrt{\Lambda_{11}(\lambda_{11}\Lambda_{11} - \Lambda)\lambda_{11}}} = \sqrt{\frac{\lambda_{11}\Lambda_{11} - \Lambda}{\lambda_{11}\Lambda_{11}}} = \sqrt{1 - \frac{\Lambda}{\lambda_{11}\Lambda_{11}}}$$

Hence

$$\rho_{1(23...n)} = \sqrt{1 - \frac{\Lambda}{\lambda_{11}\Lambda_{11}}} = \sqrt{1 - \frac{P}{P_{11}}} \qquad \text{(A. 121)}$$

for general application in n-dimensions.