Table 4 Computation time summary

To solve Eq. (3) directly by Gauss elimination	5.454 sec
To solve with approximate method	0.653 sec
Details of approximate method	
to reduce stiffness matrix	0.619 sec
to reduce load vector	0.026 sec
to solve reduced equation	0.004 sec
to assemble solution	0.004 sec

of various stages of the design sequence can be used as basic designs. There is no theoretical reason why there must be as many basic designs as there are design variables; although there is a certain intuitive appeal to having these numbers on the same order.

In many optimization applications, the most time-consuming part consists of a one-dimensional minimization, in which a number of analyses may be necessary along a "line" in the design hyperspace, and the useful basic design sets can obviously be restricted to points on this line.

It should be noted that the matrix products indicated in Eq. (7) can be performed without the complete assembly of the $\mathbf{K}_N$ matrix. This can be done in the case of finite element models with an element-by-element technique. In other cases the usually sparse matrices of structural analysis can be multiplied by matrix manipulation routines which take advantage of the zeros. None of these techniques were utilized in obtaining the results presented here.

Calculation of Theoretical Equilibrium Nozzle Throat Conditions When Velocity of Sound is Discontinuous

Sanford Gordon*
NASA Lewis Research Center, Cleveland, Ohio

1. Introduction

It is generally a routine matter to determine theoretical throat conditions (such as temperature ratio and pressure ratio) in a De Laval nozzle assuming one-dimensional, isentropic, and equilibrium expansion.[1] However, the solution of throat conditions may be considerably more difficult when two condensed phases of the same species exist simultaneously in the vicinity of the throat. The difficulty arises due to a discontinuity in the velocity of sound which occurs when, during expansion, there is a transition from one condensed phase of a species to two condensed phases of that species. If this discontinuity exists in the vicinity of the throat, then usual procedures for determining throat conditions may either give inaccurate results or become impossible to use.

This Note first presents a brief summary of the equations and procedures which may be used to determine throat conditions for usual thermodynamic conditions. Then the special case which involves discontinuities is discussed and some new procedures are presented for obtaining throat conditions for this special case.

2. Usual Procedures for Obtaining Throat Conditions

For the case of a perfect gas with constant specific heat ratio γ, simple expressions exist for obtaining temperature ratio and pressure ratio at the throat.[2] For the case of a dissociating gas, where γ is not constant, throat conditions require considerably more calculations. Equilibrium compositions and thermodynamic and flow properties such as temperature, velocity, and area per unit mass flow rate must be determined for several pressures in the vicinity of the throat.[1] Then, by interpolation or iteration, the pressure must be found for which area is minimum or, equivalently, for which the velocity of flow equals the velocity of sound (Mach number = 1).

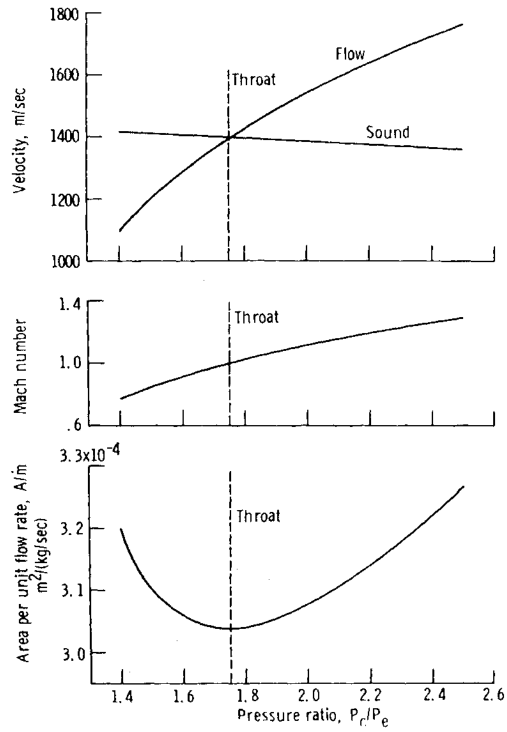

Fig. 1 Some parameters as functions of pressure ratio in vicinity of nozzle throat for typical rocket propellant.

The two methods by which throat conditions may be determined are illustrated in Fig. 1. This figure shows curves of the velocity of flow u, velocity of sound a, Mach number, and area/unit mass flow rate $A/\dot{m}$ that were obtained from theoretical equilibrium calculations of a typical rocket propellant. It is clear that throat occurs where $u = a$ (Mach number = 1) or where $A/\dot{m}$ is a minimum. This result depends on $A/\dot{m}$ and its derivative being continuous.

Equations for the determination of u, a, and $A/\dot{m}$ are given in Refs. 1 and 3. These equations, in somewhat different form, are

$$a_S = (\gamma_S nRT)^{1/2} \quad (1)$$

$$u = 2(h_c - h)^{1/2} \quad (2)$$

$$A/\dot{m} = 1/\rho u \quad (3)$$

where

$$\gamma_S \equiv (\partial \ln P/\partial \ln \rho)_S = -\gamma/(\partial \ln v/\partial \ln P)_T \quad (4)$$

$$\gamma \equiv c_P/c_V \quad (5)$$

and n is the number of moles/unit mass (reciprocal of molecular weight), R is a gas constant, T is temperature, h is enthalpy/unit mass, ρ is density, v is volume/unit mass, c_P is the specific heat at constant pressure, and c_V is the specific heat at constant volume. The subscript c refers to combustion conditions and the subscript S refers to constant entropy.

Equation (1) is obtained by combining the expression for the ideal equation of state

$$P = \rho nRT \quad (6)$$

Received May 4, 1970. Author wishes to thank B. J. McBride for assistance in obtaining the performance data.

* Head, Thermodynamic Section, Physics and Chemistry Division. Member AIAA.

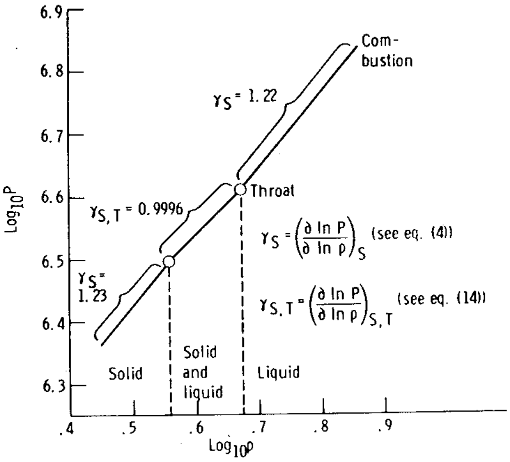

Fig. 2 Effect of Al_2O_3 phase changes on analytical and graphical values of slope γ_S or $\gamma_{S,T}$.

with the relationship for velocity of sound

$$a_S^2 = (\partial P/\partial \rho)_S = (P/\rho)(\partial \ln P/\partial \ln \rho)_S \tag{7}$$

3. Thermodynamic Derivative Discontinuities

When two condensed phases of a species coexist, the system temperature remains at the transition temperature even though other system changes may be occurring such as changes in pressure or composition. In this situation, thermodynamic derivatives with respect to temperature are not defined at the transition point. For example, $c_P = (\partial h/\partial T)_P$ or $c_V = (\partial e/\partial T)_V$ cannot be evaluated when temperature is constant. Hence, Eq. (4) cannot be used to obtain γ_S and Eq. (1) cannot be used to obtain the velocity of sound. For the condition of constant temperature and constant entropy, the following alternate expression for velocity of sound applies:

$$a_{S,T} = (\gamma_{S,T} nRT)^{1/2} \tag{8}$$

where

$$\gamma_{S,T} \equiv (\partial \ln P/\partial \ln \rho)_{S,T} \tag{9}$$

An expression for $(\partial \ln P/\partial \ln \rho)_{S,T}$ will now be derived. I will assume the equation of state for ideal gases [Eq. (6)] to be correct even when small amounts of condensed species (up to several percent by weight) are present. That is, the condensed species are assumed to occupy a negligible volume and exert a negligible pressure compared to the gaseous species. No interactions among phases are assumed to exist. In the variables v, ρ, and n, the volume and moles refer to gases only, while mass is for the entire mixture including condensed species. For example, n = moles gas/total mass.

From Eq. (6), assuming constant entropy and constant temperature,

$$(\partial \ln P/\partial \ln \rho)_{S,T} = 1 + (\partial \ln n/\partial \ln \rho)_{S,T} \tag{10}$$

The total differential of the logarithm of n, considered as a function of P and T, is

$$d \ln n = (\partial \ln n/\partial \ln P)_T d \ln P + (\partial \ln n/\partial \ln T)_P d \ln T \tag{11}$$

For constant S and T, Eq. (11) gives

$$(\partial \ln n/\partial \ln \rho)_{S,T} = (\partial \ln n/\partial \ln P)_T (\partial \ln P/\partial \ln \rho)_{S,T} \tag{12}$$

Substituting Eq. (12) into Eq. (10) gives

$$(\partial \ln P/\partial \ln \rho)_{S,T} = 1 + (\partial \ln n/\partial \ln P)_T (\partial \ln P/\partial \ln \rho)_{S,T}$$

Table 1 Theoretical equilibrium rocket performance with discontinuities at the throat (propellant; % by weight: Al, 10.8; CH_2, 19.2; NH_4ClO_4, 70)

	Combustion chamber	First throat estimate	Second throat estimate	Throat	Subsonic expansion		Supersonic expansion			
Pressure ratio P_c/P	1.0000	1.7806	1.6151	1.6815	1.4	1.6	1.8	2.0	2.2	2.5
Pressure P, N/m²	6.8947×10^6	3.8721×10^6	4.2688×10^6	4.1003×10^6	4.9248×10^6	4.3092×10^6	3.8304×10^6	3.4474×10^6	3.1340×10^6	2.7579×10^6
Temperature T, °K	2540	2315	2332	2315	2393	2336	2315	2315	2315	2262
Density ρ, kg/m³	7.2049	4.4433	4.8628	4.7052	5.4659	4.9003	4.3954	3.9557	3.5960	3.2395
n, kg-mole/kg	0.045311	0.045276	0.045277	0.045275	0.045285	0.045277	0.045276	0.045278	0.045280	0.045274
$(\partial \ln v/\partial \ln P)_T$	−1.00091	−1.00044	−1.00046	−1.00044	−1.00057	−1.00047	−1.00044	−1.00045	−1.00046	−1.00038
$(\partial \ln v/\partial \ln T)_P$	1.0170	...	1.0086	...	1.0107	1.0088	...	...	1.0092	1.0076
Specific heat c_P, joule/kg-°K	2191.5	...	2090.5	...	2116.7	2092.1	...	...	2095.2	2069.0
Isentropic exponent γ_S or $\gamma_{S,T}$	1.2149	0.9996	1.2236	...	1.2212	1.2234	0.9996	0.9995	1.2233	1.2260
Velocity of sound a_S or $a_{S,T}$, m/sec	1078.2	933.3	1036.4	...	1048.9	1037.2	933.3	933.3	1032.5	1021.6
Velocity of flow u, m/sec	0	1024.5	937.7	974.6	790.6	928.9	1033.7	1119.0	1190.9	1280.0
Mach number	0	1.098	0.905	...	0.754	0.896	1.108	1.199	1.153	1.253
Flow rate $A/\dot{m}$, m²/(kg/sec)	∞	0.0002197	0.0002193	0.0002181	0.0002314	0.0002197	0.0002201	0.0002259	0.0002335	0.0002412
Mole fraction $Al_2O_3(l)$	0.04192	0.03320	0.04218	0.04219	0.04213	0.04218	0.03150	0.01496	0	0
Mole fraction $Al_2O_3(s)$	0	0.00900	0	0.00001	0	0	0.01070	0.02724	0.04220	0.04224

or

$$\gamma_{S,T} \equiv \left(\frac{\partial \ln P}{\partial \ln \rho}\right)_{S,T} = \frac{1}{1 - (\partial \ln n/\partial \ln P)_T} = \frac{-1}{(\partial \ln v/\partial \ln P)_T} \tag{13}$$

Therefore, for the special case of constant entropy and constant temperature,

$$\gamma_{S,T} = -1/(\partial \ln v/\partial \ln P)_T \tag{14}$$

4. Numerical Example of Discontinuities

In order to numerically illustrate these derivatives and subsequent throat calculations, rocket performance calculations were made for a solid rocket propellant containing the following mass percents of ingredients: Al, 10.8; CH_2, 19.2; and NH_4ClO_4, 70.0. The chamber pressure was 6.8947×10^6 N/m^2 (1000 psia), and equilibrium composition was assumed during isentropic expansion to various exit pressures. The condensed species were assumed to travel at the local gas velocity. The results are given in Table 1. For brevity, mole fractions of the gaseous species have been omitted. The values in Table 1 are in the International System of Units (S.I.).[4] The gas constant required in Eq. (1) for this set of units is R = 8314.34 joule/(kg-mole)(°K).[4]

Figure 2 shows a plot of log P vs log ρ using data from Table 1. In this figure, the combustion point is on the right and expansion is proceeding from right to left. The curve is shown as three line segments corresponding to the three indicated conditions of the condensed phases. When just one condensed phase is present (either liquid or solid), the slope of the curve is about 1.225. However, in the region where both liquid and solid are present (where temperature is constant at melting point of 2315°K) the slope of the curve is about 0.9996. The slope can be obtained both graphically and analytically. The graphical values agree to all places shown with the analytical values given in Table 1 which were calculated from either Eq. (4) or (14).

The abrupt change in the log P vs log ρ slope (indicated by the difference between γ_S and $\gamma_{S,T}$) is caused by the abrupt change in the slope of temperature with pressure at the melting point. The change in slope from γ_S to $\gamma_{S,T}$ causes a similar abrupt change from a_S [Eq. (1)] to $a_{S,T}$ [Eq. (8)]. These changes are shown in Fig. 3 which presents curves of the variables which enter into the calculation of velocity of sound.

Figure 4 presents the same parameters as Fig. 1; however, Fig. 4 is for the case with discontinuities in velocity of sound.

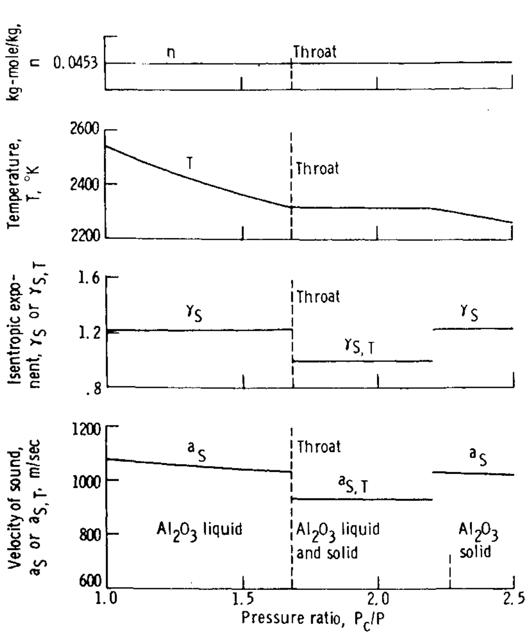

Fig. 3 Factors in velocity of sound equation.

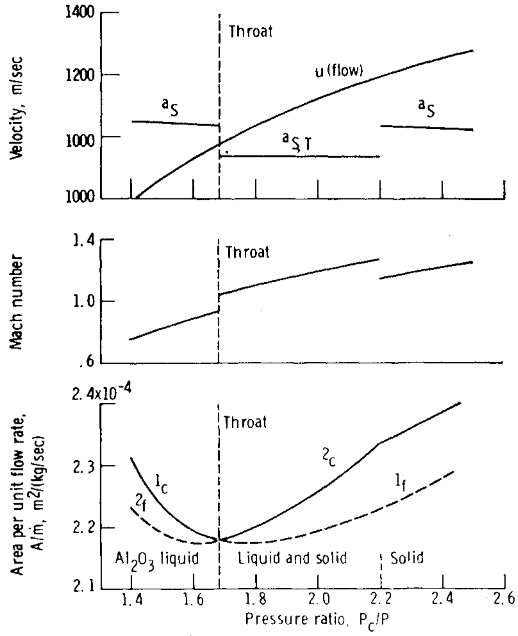

Fig. 4 Discontinuities in theoretical rocket performance parameters in vicinity of throat due to Al_2O_3 phase.

It is clear from Fig. 4 that there is no pressure ratio for which velocity of flow equals velocity of sound (no Mach number 1). Therefore, for this situation, it is obviously not possible to use any procedure which seeks the pressure ratio for which Mach number is 1.

Although one might consider usual fitting methods to locate the minimum $A/\dot{m}$, these methods might give poor results when discontinuities in slope are present. The reason for this is made clearer by an examination of the $A/\dot{m}$ curve in Fig. 4.

In Fig. 4, the solid curve labeled 1_c and 2_c represents correct thermodynamic equilibrium conditions. The region of curve 1_c includes the liquid phase of Al_2O_3, while curve 2_c includes both liquid and solid Al_2O_3 between pressure ratios of 1.6815 and 2.2 and the solid phase for pressure ratios greater than 2.2. The dashed curve 1_f is a smooth continuation of curve 1_c but represents a false thermodynamic condition. The false condition was obtained by not permitting a phase change to occur in the calculations. This was done by not permitting the solid phase of Al_2O_3 to exist as a possible species and permitting the liquid phase to exist at all temperatures below the melting point. The dashed curve 2_f is a smooth continuation of curve 2_c but also represents a false thermodynamic condition. This false condition is obtained if the solid phase is permitted to coexist (in negative amounts) with the liquid phase above the melting point.

Curves 1 and 2 both have their minimums at fictitious equilibrium conditions occurring at considerably different pressure ratios (1.61 and 1.79). The minimum value of $A/\dot{m}$ for correct equilibrium conditions is at the intersection of curves 1 and 2. The solid curve representing these conditions (1_c and 2_c) has a discontinuous slope at the minimum. For this reason, usual fitting methods based on a continuous slope might give poor results in locating the minimum.

5. Special Methods of Obtaining Throat Conditions

Two methods of obtaining throat conditions were tried for the special situation of discontinuities in velocity of sound at the throat. One method generates a separate expression for each side of the $A/\dot{m}$ curve as a function of pressure ratio and solves for their point of intersection (Fig. 4). A second method, which I prefer, locates the pressure ratio at which the solid phase just begins to appear. This method is described in Step 3 in the following suggested 3-step procedure for obtaining throat pressure ratio.

Steps 1 and 2 are to be used for all throat calculations while Step 3 is to be used only for the special case when discontinuities are present at the throat.

A suggested procedure

Step 1: Obtain an initial estimate for throat pressure ratio from the approximate formula

$$P_c/P_t = [(\gamma_S + 1)/2]^{\gamma_S/(\gamma_S - 1)} \quad (15)$$

using the value of γ_S corresponding to the combustion conditions. For the example in Table 1, using $\gamma_S = 1.2149$, Eq. (15) gives as a first estimate $P_c/P_t = 1.7806$. Equilibrium calculations for this estimated pressure ratio are shown in the second column of Table 1. The throat temperature for this first estimate is 2315°K (the melting point of Al_2O_3) with mole fractions of $Al_2O_3(l) = 0.03320$ and $Al_2O_3(s) = 0.00900$.

Step 2: Obtain a second estimate for throat pressure ratio. If the method of Ref. 1 is used, the next estimate is $P_c/P_t = 1.6151$. At this pressure ratio, T_t is 2332°K which is above the melting point of 2315°K and no $Al_2O_3(s)$ is present. The sequence of Steps 1 and 2 (namely, liquid and solid at one estimate of throat pressure ratio and liquid only at the next estimate) indicates that discontinuities exist at the throat.

Step 3: Estimate the pressure ratio at the melting point where the solid phase just begins to appear. This may be done by using the following expression:

$$\ln P_t = \ln P + (\partial \ln P/\partial \ln T)_S(\ln T_{m.p.} - \ln T) \quad (16)$$

where[3]

$$(\partial \ln P/\partial \ln T)_S = c_P/nR(\partial \ln v/\partial \ln T)_P \quad (17)$$

In Eqs. (16) and (17), the values for the right hand side are for the previous point, $P_c/P_t = 1.6151$ [no $Al_2O_3(s)$]. Equation (17) gives a value $(\partial \ln P/\partial \ln T)_S = 5.5059$. This value in Eq. (16) gives a final throat estimate of $P_t = 4.1003 \times 10^6$ N/m^2 or $P_c/P_t = 1.6815$. At this pressure ratio, equilibrium calculations gave $T = 2315$°K and a mole fraction of 0.00001 for $Al_2O_3(s)$, as may be seen in Table 1 in the column labeled "Throat."

6. Discussion

For the assumed model, the correct throat pressure ratio giving zero mole fraction for $Al_2O_3(s)$ at $T = 2315$°K is 1.6814. Therefore, for this example, the suggested method located the throat pressure ratio to within 0.0001 (0.006%) of the correct value which is in excellent agreement. For several other cases that were tried and that involved a much longer extrapolation in Eq. (16) than in this case, the throat pressure ratio was within 0.0005 (0.03%) of the correct pressure ratio which is still excellent.

The calculation of throat conditions for the special circumstances discussed in this paper has been incorporated as part of a general computer program for chemical equilibrium calculations. The program, which includes several applications, is available from the author.

References

[1] Zeleznik, F. J. and Gordon, S., "A General IBM 704 or 7090 Computer Program for Computation of Chemical Equilibrium Compositions, Rocket Performance, and Chapman-Jouguet Detonations," TN D-1454, 1962, NASA.

[2] Shapiro, A. H., *Dynamics and Thermodynamics of Compressible Fluid Flow*, Vol. 1, Ronald Press, New York, 1953, p. 84.

[3] Zeleznik, F. J. and Gordon, S., "Calculation of Complex Chemical Equilibria," *Industrial and Engineering Chemistry*, Vol. 60, No. 6, June 1968, pp. 27–57; also *Applied Thermodynamics*, American Chemical Society Publications, 1968, p. 303.

[4] Mechtly, E. A., *The International System of Units, Physical Constants and Conversion Factors*, SP-7012, NASA, 1969.

Structural Optimization of a Panel Flutter Problem

Raymond H. Plaut*
Brown University, Providence, R. I.

Nomenclature

a_i	= modal amplitudes
b	= segment length
c	= panel length
$D(X)$	= panel stiffness
D_o	= reference stiffness of uniform panel
g_o	= aerodynamic damping parameter = $\rho Uc^2(M^2 - 2)/[(M^2-1)^{3/2}(D_o m_o)^{1/2}]$
M	= Mach number
$m(X), m_i$	= panel mass per unit length
$\bar{m}(X), \bar{m}_i$	= optimal values of m, m_i
m_o	= reference mass of uniform panel
P	= midplane compressive load
p	= dimensionless load = Pc^2/D_o
p_o	= critical value of p for flutter
$\bar{p}, \bar{p}_o$	= approximate critical values of p
T	= time
t	= dimensionless time = $T(D_o/m_o)^{1/2}/c^2$
U	= speed of supersonic flow
$\bar{W}$	= total weight of optimum panel
W_o	= total weight of reference uniform panel
$W(X,T)$	= panel deflection
$w(x,t)$	= dimensionless panel deflection = W/c
$w_i(x)$	= deflection modes
X	= coordinate along length
x	= dimensionless coordinate = X/c
α^2, β^2	= parameters relating mass and stiffness
γ	= $[(1-\alpha^2)/\beta^2]^{1/2}$
$\delta(x), \delta_i$	= dimensionless panel stiffness; $\delta = D/D_o$
$\mu(x), \mu_i$	= dimensionless mass; $\mu = m/m_o$
$\bar{\mu}(x), \bar{\mu}_i$	= optimal values of μ, μ_i
θ	= frequency parameter
λ_o	= dynamic pressure parameter = $\rho U^2 c^3/[D_o(M^2 - 1)^{1/2}]$; $\lambda_o > 125$
ρ	= density of air
$(\ )'$	= $d(\ )/dx$

Introduction

Recent reviews by Ashley[1] and Dowell[2] have described the present status of research on panel flutter. A new development concerns the structural optimization of panels in order to minimize the panel weight while satisfying certain flutter requirements. This problem has been considered by Turner[3] and by McIntosh, Weisshaar, and Ashley.[4] An approximate method for obtaining the optimal panel design is proposed here, and calculations are carried out for a panel with segment-wise constant mass distribution. The results, although only approximate, indicate that significant savings in weight may be possible with the use of nonuniform panels.

Analysis

Consider a flat elastic panel of infinite span, as shown in Fig. 1, subjected to a supersonic flow over one side and a uniform midplane compressive load P. The equation of motion based on first-order theory is given by[5]

$$\frac{\partial^2}{\partial X^2}\left[D(X)\frac{\partial^2 W}{\partial X^2}\right] + m(X)\frac{\partial^2 W}{\partial T^2} + P\frac{\partial^2 W}{\partial X^2} + \frac{\rho U^2}{(M^2-1)^{1/2}}\left[\frac{\partial W}{\partial X} + \frac{(M^2-2)}{U(M^2-1)}\frac{\partial W}{\partial T}\right] = 0 \quad (1)$$

Received July 13, 1970; revision received July 24, 1970. This paper was supported in part by the U. S. Army Research Office—Durham and in part by the United States Navy under Grant NONR N00014-67-A-0191-0009.

* Assistant Professor of Applied Mathematics and Engineering (Research).