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COMPUTER PROGRAMS TO CALCULATE CHEMICALLY REACTING FLOW IN AXIS--ETC(U)
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Computer Programs to Calculate
Chemically Reacting Flow
in Axisymmetric Nozzles

John M. Cousins

May 1978

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9 Technical Report No. 84
Approved February 1978

6 COMPUTER PROGRAMS TO CALCULATE CHEMICALLY REACTING FLOW
IN AXISYMMETRIC NOZZLES.

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by

10 Jane M. Cousins

12 57 p.

SUMMARY

This report describes a set of computer programs which calculates the inviscid two-dimensional expansion of gaseous exhaust mixtures through rocket nozzles. Equilibrium chemistry in the combustion chamber and as far as the nozzle throat is assumed, whilst finite rate or frozen chemistry may be applied from the throat onwards. The transonic flow field is calculated by the method of streamline curvature and the flow in the supersonic region of the nozzle is solved by the method of characteristics.

The theory on which the programs are based is summarised and a comprehensive user's guide is included. A sample calculation is presented.

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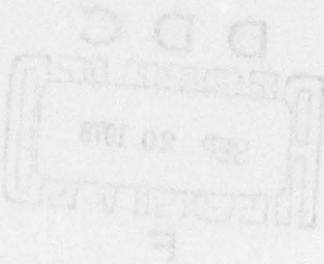
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1 INTRODUCTION

The computer programs described provide means of calculating the steady, inviscid two-dimensional expansion of a gaseous mixture through an axisymmetric rocket exhaust nozzle (Fig. 1), allowing for the effects of chemical reaction rates during expansion of the exhaust gas.

The set of programs consists of:

- (a) ODN0Z (one-dimensional nozzle expansion), which permits the rapid calculation of the equilibrium temperature and composition inside a rocket motor combustion chamber, and provides an axial profile of gas composition, temperature and pressure along the nozzle with the assumption of equilibrium chemistry (infinite reaction rates). Tables of flow properties (x, T, ρ, m, M) and species mole fractions X_i are constructed.
- (b) TRANOZ (transonic nozzle flow), which calculates an average expansion coefficient γ from the above tables, and assuming constant stagnation conditions calculates the axisymmetric, transonic flow field by the method of streamline curvature. An initial constant property data line is constructed for input to
- (c) SUPERNOZ (supersonic nozzle program), which calculates the flow in the supersonic region of the nozzle by the method of characteristics, with either a frozen chemical composition (zero reaction rates) or taking into account the finite, non-zero rates of chemical reactions. It provides accurate exit plane conditions which may be used as input to an exhaust plume analysis program, such as the Rocket Exhaust Plume program (REP)¹ or the Base Flow program (BAFL)².

The sequence of calculations is illustrated in Fig. 1.

The programs already represent a significant advance over those currently used at PERME for calculating the flow from the combustion chamber to the nozzle exit plane³, in that they can treat two-dimensional flow, and they are to be further enhanced by including the non-equilibrium effects of gas/particle flow. These have already been incorporated into the transonic flow program without chemistry⁴, and the full two-dimensional, two-phase flow treatment should shortly be available.

This report serves primarily as a program user's guide, but also contains a summary of the theoretical basis of the programs. The governing equations are included and the method of solution for each of the three programs is described.

The data and results of a sample calculation are presented. The results are all given in SI units, and the working units for the fluid dynamic equations are SI. In the chemical equations most of the variables are non-dimensional. The programs are written in FORTRAN IV, permitting their use on all standard computers and are designed for easy use, requiring only specification of the propellant composition, pressure and enthalpy, nozzle geometry, thermodynamic data and the chemical reaction scheme with rate coefficients.

2 ONE-DIMENSIONAL EXPANSION WITH EQUILIBRIUM CHEMISTRY

The program ODN0Z is a modified version of NEWFEC³, with the addition of a cubic spline fitting routine, which permits a contoured nozzle from the throat onwards. Most of the theory and methods used in the program are taken from Ref. 5, any differences in the chemical treatment being described in Ref. 3.

2.1 Chamber calculation

The gaseous propellant mixture is made up of s chemical species, of which c are either chemical elements (H, O, N, etc.), or linearly independent combinations of the chemical elements (H₂, O₂, N₂, etc.), and $s-c$ are dependent species formed by simple combinations of the c independent species. The system is specified through the matrix Λ , in which the element α_{ij} represents the number of moles of independent species j per mole of dependent species i . The number of moles of the fundamental species per unit mass of the unreacted mixture q'_j , $j=1, 2, \dots, c$, must be given. The conservation of chemical elements and global mass conservation are expressed by the equations

$$X_j = q_j - \sum_{i=c+1}^s \left[\alpha_{ij} - q_j \left(\sum_{k=1}^c \alpha_{ik} - 1 \right) \right] X_i \quad j=1, 2, \dots, c \quad (2.1)$$

where X_i , $i=1, 2, \dots, s$ is the mole fraction of species i and

$$q_j = \frac{q'_j}{\sum_{j=1}^c q'_j}$$

At chemical equilibrium the dependent species concentrations are related to the concentrations of the components through the equilibrium constants in the equation:

$$X_i = K_p^i P_a \left(\sum_{k=1}^c \alpha_{ik} - 1 \right) \prod_{j=1}^c X_j^{\alpha_{ij}} \quad i=c+1, \dots, s \quad (2.2)$$

where P_a is the mixture pressure in atmospheres. The factor

$$K_p^i = \exp \left[\sum_{j=1}^c \left(\alpha_{ij} \frac{\mu_j^0}{T_n} \right) - \frac{\mu_i^0}{T_n} \right]$$

is the equilibrium constant based on partial pressure for species i , T_n is the mixture temperature T , normalised by the combustion chamber temperature T_0 , so that in the chamber $T_n = 1$, and μ_i^0 is the normalised chemical potential of species i .

Substitution from equation (2.2) into equation (2.1) for the X_i , $i=c+1, \dots, s$, reduces equation (2.1) to a set of c simultaneous equations which may be solved iteratively for the equilibrium concentrations of the independent species at a given pressure P_a and temperature T . The chamber temperature T_0 is not known initially and so the specific enthalpy H_0 , which may be readily determined from the heats of formation of the constituent compounds, is specified and the solution is found by iteratively varying the temperature until the mixture enthalpy H matches the specific enthalpy.

2.2 Equilibrium expansion

The equations of continuity and conservation of momentum and energy for an inviscid gas are

$$\rho u A = \text{constant} \quad (2.3)$$

$$u \, du + \frac{1}{\rho} \, dP = 0 \quad (2.4)$$

$$H + \frac{1}{2} u^2 = H_0 = \text{constant} \quad (2.5)$$

where u is the velocity, ρ is the density and A is the cross-sectional area of the nozzle normalised by the throat area.

The equation of state for an ideal gas is

$$p = \frac{\rho T R}{m} \quad (2.6)$$

where m is the molecular weight and R is the universal gas constant.

The energy and momentum equations may be used to show that the inviscid expansion of a flow in chemical equilibrium is an isentropic process. The molar entropy of a chemically reacting gas mixture is given by

$$s = \frac{1}{m} \left\{ \sum_{j=1}^s X_j s_j^0 - \sum_{j=1}^s X_j \ln X_j - \ln P_a \right\} = S_0 \quad (2.7)$$

where s_j^0 is the molar entropy of species j at 1 atmosphere. Equations (2.1) and (2.7) now give a set of $c+1$ simultaneous equations for determining the composition and pressure of the mixture at a given temperature. The equilibrium solution is obtained at successive temperature intervals, computing the flux, ρu , at each point from equations (2.5) and (2.6). The maximum flux and the corresponding temperature determine the throat conditions and the critical mass flow for the equilibrium expansion. After the mass flow has thus been found the chemical composition and aerodynamic variables at given axial stations may be calculated from equations (2.1) to (2.7), and tables of flow properties (x, T, ρ, m, M) and species mole fractions X_i , $i=1, 2, \dots, s$ are constructed for input to the next stage of the calculation. The equilibrium exit plane conditions are also given.

3 TWO-DIMENSIONAL TRANSONIC FLOW

In the solution of the two-dimensional equations for flow through a convergent/divergent nozzle with a transonic region, many mathematical difficulties are encountered in the region of transition from subsonic to supersonic flow. Although the transition is smooth the properties in the two regions are quite different. In the subsonic region the governing equations are elliptic, whereas in the supersonic region they are hyperbolic. The supersonic flow field may be solved by the method of characteristics, but accurate initial line data are needed to start the calculation. Since the flow near the nozzle throat may be far from one-dimensional, the sonic velocity at the wall being reached well upstream of the throat, while that at the axis is reached downstream of the

throat (see, for example, Fig. 2), a method of solution which describes the properties of both subsonic and supersonic flow segments must be devised. A further difficulty is that the mass flux is not known and must be calculated. When chemical reactions are taken into account the problem becomes even more complex and it is thus necessary to construct by approximate means an initial line suitable for starting the method of characteristics solution of the flow field in the supersonic domain.

In TRANOZ, an effective expansion coefficient is computed by

$$\bar{\gamma} = \frac{\ln (P_L / P_o)}{\ln (\rho_L / \rho_o)}$$

where L refers to the last entry in the table constructed by ODNOZ and o denotes the chamber value. A mean molecular weight is found from

$$\bar{m} = \frac{1}{2} (m_o + m_L)$$

and the stagnation conditions are assumed to remain constant at the chamber values.

There are several ways of solving the equations of transonic, axisymmetric flow, but most are restricted to nozzles of a particular shape and with a throat wall radius of curvature greater than (at least) the throat radius. The method adopted in TRANOZ is based on that described by Stow⁶, which was developed from the "streamline curvature" method used for subsonic flows in turbomachines (see, for example, Marsh⁷). It is an iterative procedure which may be applied to nozzles of general geometry and which is convergent and stable, even for nozzles with a throat wall radius of curvature smaller than the throat radius.

When the transonic flow field has been calculated, the wall Mach number at a specified point is found and a table of (x,r,θ) values corresponding to this value of M on each streamline is constructed, to start the supersonic solution (see Fig. 2). The point chosen is usually the throat wall point, since this permits a finite rate chemical treatment as far upstream as possible. The initial line thus constructed is an approximation to the constant pressure surface for a Mach number of slightly greater than unity, along which it is reasonable to assume that a constant expansion coefficient can be used. The other gas properties corresponding to this Mach number are obtained by interpolation from the tables constructed by ODNOZ.

3.1 Method of streamline curvature

The equations governing the steady axisymmetric motion of an inviscid compressible fluid are, in the co-ordinates of Fig. 3, where x and r are normalised by the throat radius r^* :

continuity

$$\frac{\partial}{\partial x} (r\rho u) + \frac{\partial}{\partial r} (r\rho v) = 0 \quad , \quad (3.1)$$

conservation of momentum

$$u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial r} = - \frac{1}{\rho} \frac{\partial P}{\partial x} \quad (3.2)$$

$$u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial r} = - \frac{1}{\rho} \frac{\partial P}{\partial r} \quad . \quad (3.3)$$

Equation (3.1) implies the existence of a stream function ψ satisfying

$$\frac{\partial \psi}{\partial r} = r\rho u \quad , \quad \frac{\partial \psi}{\partial x} = - r\rho v$$

or

$$\psi(x, r) = \int^r (r\rho u)_{x=\text{constant}} dr + \text{constant} \quad . \quad (3.4)$$

By introducing the speed of sound, defined by $c = (\partial P / \partial \rho)^{1/2}$, equations (3.1) to (3.3) may be combined to obtain the radial equilibrium equation, relating the static pressure field to the streamline geometry. Detailed derivations are given in Refs 4 and 6, but only the final equation is reproduced here*:

$$\left(1 - \frac{u^2}{c^2} \sec^2 \theta \right) \frac{1}{\rho} \left(\frac{\partial P}{\partial r} \right)_x = - u^2 \left(1 - \frac{u^2}{c^2} \right) \left(\frac{\partial \tan \theta}{\partial x} \right)_\psi + u^2 \tan \theta \left(\frac{\partial \tan \theta}{\partial r} \right)_x + \frac{u^2 \tan^2 \theta}{r} \quad . \quad (3.5)$$

*Subscripts x , ψ imply differentiation along a line of constant x or ψ .

The term $\left(\frac{\partial \tan \theta}{\partial x} \right)_{\psi}$ is referred to as the "curvature" of a streamline.

3.2 Solution procedure

Equation (3.5) is solved iteratively along axial stations in the flow. Each axial station is divided into a number of radial mesh points (see Fig. 3) and the equation is applied at points mid-way between the mesh points. It is assumed that an estimate for the flow pattern is available from a previous iteration, so that equation (3.5) becomes an ordinary differential equation in the static pressure.

To begin the iterative procedure an approximation is made to the mid-radial pressure and the shape of the streamlines from one-dimensional considerations, and equation (3.5) is integrated radially to obtain the pressure profile. The mass flux is determined from equation (3.4) and the mid-radial pressure is varied until the calculated mass flux agrees with the true mass flux. All the axial stations are solved in this way, and the other flow variables are evaluated from isentropic relationships. A new approximation to the streamline geometry is made and the calculation is repeated until the solution converges.

In the case of choked internal flow the mass flux must be determined. This is calculated at the throat in each iteration by choosing the mid-radial pressure which maximises the mass flow through the throat. This is equivalent, in one-dimensional flow, to finding the sonic point. The calculation is then progressed upstream and downstream of the throat using this mass flux.

At axial stations upstream and downstream of the throat two possible isentropic solutions exist. These correspond to the subsonic and supersonic solutions of one-dimensional flow, although in the two-dimensional case the flow can be mixed in the radial direction. Upstream of the throat the equivalent of the one-dimensional subsonic solution is chosen and for rocket nozzles, where the back pressure is such that the flow becomes supersonic downstream of the throat, the equivalent of the one-dimensional supersonic solution is chosen at stations downstream of the throat.

In practice the iterative procedure is conditionally stable and relaxed values of the calculated slope and "curvature" must be used to ensure convergence. For example

$$(\tan\theta)_{\text{used}}^n = (\tan\theta)_{\text{used}}^{n-1} + \text{relaxation factor} \times \left[(\tan\theta)_{\text{found}}^n - (\tan\theta)_{\text{used}}^{n-1} \right]$$

where $(\tan\theta)^n$ represents the n th approximation to $\tan\theta$ and the subscripts "found" and "used" refer to the value calculated and that used in the next iteration. The relaxation factor depends upon the nozzle geometry, as does the number of steps required, convergence being assumed when the change in the flow parameters between successive iterations is smaller than some desired degree of accuracy.

4 SUPERSONIC METHOD OF CHARACTERISTICS SOLUTION WITH NON-EQUILIBRIUM CHEMISTRY

The computer program SUPERNOZ calculates the inviscid two-dimensional frozen or non-equilibrium expansion of a gaseous mixture through the supersonic region of a rocket exhaust nozzle by the method of characteristics. Characteristics are lines, like streamlines, along which the partial derivatives may be grouped together in such a manner that they form ordinary derivatives in the direction of the characteristics. For supersonic flow the characteristics are real and coincident with the Mach lines; thus, for any point P in the flow the angle between the tangent to a characteristic and the tangent to a streamline is the Mach angle α . For every such point P in the flow there are two characteristic lines, referred to as the left and right running characteristics (Fig. 4).

With the initial data line constructed by TRANOZ as a starting point, the characteristic equations governing the fluid dynamic variables are integrated via an explicit integration technique⁸, while the chemical relaxation equations are integrated using an implicit integration method³ to ensure numerical stability in near-equilibrium flows. In explicit numerical solutions the solution is calculated step by step from the given differential equation and known initial conditions, whereas in implicit solutions, the unknown values are bound together by a system of simultaneous equations. The fluid dynamic equations are integrated explicitly since the required integration step sizes are not stability limited, and an implicit formulation of the equations would unnecessarily complicate the calculations.

The theory on which the solution of the fluid dynamic equations is based is taken from Ref. 8 and the integration scheme for the non-equilibrium chemical equations is taken from the one-dimensional program FIRAC³.

4.1 Characteristic equations

The conservation equations governing the steady axisymmetric inviscid flow of a reacting gas mixture are, in characteristic form⁸,

$$\frac{dr}{dx} = \tan \theta \quad (4.1)$$

$$d \frac{V^2}{2} + \frac{dP}{\rho} = 0 \quad (4.2)$$

$$\frac{dP}{\gamma P} - \frac{d\rho}{\rho} = \frac{A}{\cos \theta} dx \quad (4.3)$$

$$\frac{\gamma-1}{\gamma} \frac{dP}{P} - \frac{dT}{T} = \frac{B}{\cos \theta} dx \quad (4.4)$$

$$dc_j = \frac{w_j r^*}{\rho V \cos \theta} dx \quad (4.5)$$

along streamlines, where c_j is the species mass fraction, w_j is the net species production rate and r^* is the throat radius,

$$\frac{dx}{dr} = \cot (\theta + \alpha) \quad (4.6)$$

$$\frac{dP}{P} = G \left[\left(A - \frac{\sin \theta}{r} \right) F dr - d\theta \right] \quad (4.7)$$

along left running characteristics, and

$$\frac{dr}{dx} = \tan (\theta - \alpha) \quad (4.8)$$

$$\frac{dP}{P} = -G \left[\left(A - \frac{\sin \theta}{r} \right) H dx - d\theta \right] \quad (4.9)$$

along right running characteristics, where

$$A = \frac{r^*}{PV} \left(\sum_{j=1}^s w_j \frac{R}{m_j} T - \frac{\gamma-1}{\gamma} \sum_{j=1}^s w_j h_j \right) \quad (4.10)$$

$$B = \frac{r^*}{PV} \frac{\gamma-1}{\gamma} \sum_{j=1}^s w_j h_j \quad (4.11)$$

$$V = (u^2 + v^2)^{1/2} \quad (4.12)$$

$$\theta = \tan^{-1} \left(\frac{v}{u} \right) \quad (4.13)$$

$$\alpha = \sin^{-1} \left(\frac{1}{M} \right) \quad (4.14)$$

$$M = \frac{V}{(\gamma RT)^{1/2}} \quad (4.15)$$

$$\gamma = \frac{C_p}{C_p - R/m} \quad (4.16)$$

$$F = \cos \theta - \sin \theta \cot(\theta + \alpha) \quad (4.17)$$

$$G = \frac{\gamma}{\sin \alpha \cos \alpha} \quad (4.18)$$

$$H = \cos \theta \tan(\theta - \alpha) - \sin \theta \quad (4.19)$$

The above relationships remain determinant provided that the flow is always supersonic, that is $M > 1$.

4.2 Non-equilibrium chemistry

The non-equilibrium conditions are expressed as differential forms of the conservation equations⁵:

$$\sum_{j=1}^s \left[\alpha_{jk} \frac{dy_j}{dx} \right] = 0 \quad k=1, 2, \dots, c \quad (4.20)$$

$$\frac{dy_j}{dx} = \sum_{i=1}^r \beta_{ij} P_i X_i \quad j=c+1, \dots, s \quad (4.21)$$

where γ_j is the concentration variable in moles per gram, defined by

$$\gamma_j = \frac{X_j}{m} = \frac{c_j}{m_j},$$

r is the number of reactions, and

$$\beta_{ij} = v'_{ij} - v_{ij}$$

$$P_i = \frac{r^* (.001 \rho)}{(100 u)} v_i^{-1} k_{f_i} \prod_{j=1}^s \gamma_j^{v_{ij}} \text{ mole g}^{-1}$$

$$X_i = 1 - \frac{(\rho/\rho_0)^{\beta_i}}{K_i} \prod_{j=1}^s \gamma_j^{\beta_{ij}}$$

where v_{ij} , v'_{ij} are the stoichiometric coefficients of species j in the reaction i on the reactants and products sides respectively, k_{f_i} is the forward rate coefficient of the i th reaction and K_i is the equilibrium constant of reaction i . In addition,

$$v_i = \sum_{j=1}^s v_{ij}$$

$$\beta_i = \sum_{j=1}^s \beta_{ij}.$$

4.3 Numerical integration technique

The reacting gas characteristic relationships (equations (4.1) to (4.9)) are usually integrated via second order explicit methods. However, for near-equilibrium chemistry, the explicit form of equation (4.5) requires impractically small integration step sizes to ensure stability. Thus the fluid dynamic equations ((4.1) to (4.4) and (4.6) to (4.9)), which are not stability limited to small step lengths, are integrated by explicit methods, since an implicit

formulation of the equations would unnecessarily complicate the calculations, and the chemical concentrations are found via an implicit scheme.

4.3.1 Integration of fluid dynamic equations

Consider the flow field shown in Fig. 4, where point 4 is a known back data point, points 1 and 2 are known points located on the right and left running characteristics respectively, and point 3 is the point to be calculated. Between points 3 and 4 the streamline characteristic relationships are integrated as⁸

$$r_3 = r_4 + \tan \frac{1}{2} (\theta_4 + \theta_3) (x_3 - x_4) \quad (4.22)$$

$$v_3 = \left\{ v_4^2 + \frac{2\bar{\gamma}}{\bar{\gamma}-1} \frac{p_4}{\rho_4} \left[1 - \left(\frac{p_3}{p_4} \right)^{\frac{\bar{\gamma}-1}{\bar{\gamma}}} \right] \right\}^{1/2} \quad (4.23)$$

where

$$\bar{\gamma} = \frac{\ln (p_3/p_4)}{\ln (\rho_3/\rho_4)}$$

$$\rho_3 = \rho_4 \left(\frac{p_3}{p_4} \right)^{\frac{1}{2} \left(\frac{1}{\gamma_4} + \frac{1}{\gamma_3} \right)} \exp \left[-\frac{1}{2} \left(\frac{A_4}{\cos \theta_4} + \frac{A_3}{\cos \theta_3} \right) (x_3 - x_4) \right] \quad (4.24)$$

$$T_3 = T_4 \left(\frac{p_3}{p_4} \right)^{\frac{1}{2} \left(\frac{\gamma_4-1}{\gamma_4} + \frac{\gamma_3-1}{\gamma_3} \right)} \exp \left[-\frac{1}{2} \left(\frac{B_4}{\cos \theta_4} + \frac{B_3}{\cos \theta_3} \right) (x_3 - x_4) \right] \quad (4.25)$$

Between points 1 and 3 the right running characteristic relationships are integrated as

$$r_3 = r_1 + \tan \left[\frac{1}{2} (\theta_1 + \theta_3 - \alpha_1 - \alpha_3) \right] (x_3 - x_1) \quad (4.26)$$

$$\begin{aligned}
 P_3 = P_1 \exp \left\{ - \left[\frac{1}{2} (A_1 G_1 H_1 + A_3 G_3 H_3) (x_3 - x_1) \right. \right. \\
 - \frac{1}{2} \left(\frac{G_1 H_1 \sin \theta_1}{r_1} + \frac{G_3 H_3 \sin \theta_3}{r_3} \right) (x_3 - x_1) \\
 \left. \left. - \frac{1}{2} (G_1 + G_3) (\theta_3 - \theta_1) \right] \right\} . \quad (4.27)
 \end{aligned}$$

If point 3 is an axis point, r_3 and θ_3 are zero and the indeterminate quantity $\sin \theta_3 / r_3$ is approximated by

$$\frac{\sin \theta_3}{r_3} = \frac{\tan \theta_1}{r_1 + (x_3 - x_1) \tan \theta_1} . \quad (4.28)$$

Between points 2 and 3 the left running characteristic relationships are integrated as

$$x_3 = x_2 + \cot \left[\frac{1}{2} (\theta_2 + \theta_3 + \alpha_2 + \alpha_3) (r_3 - r_2) \right] \quad (4.29)$$

$$\begin{aligned}
 P_3 = P_2 \exp \left[\frac{1}{2} (A_2 G_2 F_2 + A_3 G_3 F_3) (r_3 - r_2) \right. \\
 - \frac{1}{2} \left(\frac{G_2 F_2 \sin \theta_2}{r_2} + \frac{G_3 F_3 \sin \theta_3}{r_3} \right) (r_3 - r_2) \\
 \left. - \frac{1}{2} (G_2 + G_3) (\theta_3 - \theta_2) \right] . \quad (4.30)
 \end{aligned}$$

If point 2 is an axis point the indeterminate quantity $\sin \theta_2 / r_2$ is that quantity previously calculated for the axis point by equation (4.28).

Equations (4.27) and (4.30) can be combined to give

$$\begin{aligned}
\theta_3 = & \frac{1}{G_3 + \frac{1}{2}(G_1 + G_2)} \left[\ln \left(\frac{P_2}{P_1} \right) + \frac{1}{2}(G_1 + G_3)\theta_1 + \frac{1}{2}(G_2 + G_3)\theta_2 \right. \\
& + \frac{1}{2}(A_2 G_2 F_2 + A_3 G_3 F_3)(r_3 - r_2) \\
& - \frac{1}{2} \left(\frac{G_2 F_2 \sin \theta_2}{r_2} + \frac{G_3 F_3 \sin \theta_3}{r_3} \right) (r_3 - r_2) \\
& + \frac{1}{2}(A_1 G_1 H_1 + A_3 G_3 H_3)(x_3 - x_1) \\
& \left. - \frac{1}{2} \left(\frac{G_1 H_1 \sin \theta_1}{r_1} + \frac{G_3 H_3 \sin \theta_3}{r_3} \right) (x_3 - x_1) \right] \quad (4.31)
\end{aligned}$$

Since the above integration equations involve the flow properties at the unknown points 3, they must be solved by iteration. The iterative technique is described in Section 4.4.

4.3.2 Integration of chemical equations

The set of equations giving the increments $\delta\gamma_i$ of the concentration variables γ_i is³:

$$\begin{aligned}
\left[1 - \epsilon_1 \left(\frac{\partial f_i}{\partial \gamma_i} \right)_n \right] (\delta\gamma_i)_{n+1} - \epsilon_1 \sum_{j=1}^s \left[(1 - \delta_{ij}) \left(\frac{\partial f_i}{\partial \gamma_j} \right)_n (\delta\gamma_j)_{n+1} \right] \\
= \epsilon_2 (\delta\gamma_i)_n + \epsilon_1 \left[(f_i)_n + (\Delta x)_{n+1} \left(\frac{\partial f_i}{\partial x} \right)_n \right] \\
i=1, 2, \dots, s \quad (4.32)
\end{aligned}$$

where $f_i = \frac{d\gamma_i}{dx}$

$(\delta\gamma_i)_{n+1}$ = change in γ_i in a distance $(\Delta x)_{n+1}$ along a streamline

$(\Delta x)_{n+1} = x_{n+1} - x_n$

$$\epsilon_1 = \frac{(\Delta x)_{n+1} [(\Delta x)_{n+1} + (\Delta x)_n]}{[2(\Delta x)_{n+1} + (\Delta x)_n]}$$

$$\epsilon_2 = \frac{(\Delta x)_{n+1}^2}{(\Delta x)_n [2(\Delta x)_{n+1} + (\Delta x)_n]}$$

$$\delta_{ij} = 1, \quad i=j$$

$$= 0, \quad i \neq j$$

The partial derivatives $\frac{\partial f_i}{\partial \gamma_i}$ are determined numerically from

$$\frac{\partial f_i}{\partial \gamma_i} = \frac{f_i(\gamma_1, \gamma_2, \dots, \gamma_j + \lambda_j, \dots, \gamma_s) - f_i(\gamma_1, \gamma_2, \dots, \gamma_j - \lambda_j, \dots, \gamma_s)}{2 \lambda_j}$$

where λ_j is some small fraction of γ_j and the ordinary derivatives $\frac{df_i}{dx}$ are found by solving equations (4.20) and (4.21). Equation (4.21) cannot be used at the initial data line, where the flow is in equilibrium, so an additional equation is obtained for starting the solution by differentiating equation (2.2), to give

$$\frac{1}{\gamma_i} \frac{d\gamma_i}{dx} - \sum_{j=1}^c \frac{\alpha_{ij}}{\gamma_j} \frac{d\gamma_j}{dx} + \left\{ \sum_{j=1}^c \left[\frac{\alpha_{ij}}{T_n} \left(\frac{h_j}{T_n} - 1 \right) \right] - \left(\frac{h_i}{T_n} - \frac{1}{T_n} \right) \right\} \frac{dT_n}{dx} - \left\{ \sum_{j=1}^c \alpha_{ij} - 1 \right\} \frac{d \ln(\rho|\rho_0)}{dx} = 0 \quad i=c+1, \dots, s$$

where the derivatives $\frac{dT_n}{dx}$ and $\frac{d \ln(\rho|\rho_0)}{dx}$ are provided along the initial data line by TRANOZ.

4.4 Solution procedure

The characteristic mesh for the supersonic solution is shown in Fig. 4. The solid dots are known points on the back data line, and the squares represent the points to be computed. Point 2 is the point on the back data line next below point 4, and the unknown point 3 lies at the intersection between the streamline through point 4 and the left running characteristic through point 2. Point 1 is at the intersection between the right running characteristic through point 3 and the left running characteristic through point 4. Values at point 1 are determined by interpolation.

The iterative solution is started by assuming that the previously uncalculated flow variables on the right hand sides of equations (4.22) to (4.31) are equal to the values at points 4, 2 or 1 depending on whether the integration is along a streamline or a left or right running characteristic, respectively. Initial estimates of the locations of point 3 and, except for wall points, point 1 are made and the fluid dynamic variables at point 3 are found from equations (4.22) to (4.31). The species concentrations at point 3 are calculated by integration of the chemical equations, and the other properties at point 3 are found from equations (4.10) to (4.19). New estimates of the locations of points 3 and 1 are made, and the solution procedure is repeated, always using the latest computed values of the flow properties at point 3, until $r_3, x_3, \theta_3, P_3, \rho_3, T_3$ and V_3 converge to the required accuracy.

The first point to be computed is the nozzle wall point. Only two known data points are required here since, once the axial location of point 3 has been found, r_3 and θ_3 may be determined from the nozzle geometry. The internal points are then computed, starting with the point adjacent to the wall and continuing with the one immediately below it, until the nozzle axis is reached. Again, only two back points are needed here, since r_3 and θ_3 are both zero on the axis. When all the forward points have been calculated, the new data line becomes the back data line, and the computation is progressed downstream until the exit plane is reached.

4.5 Thrust calculation

When the exit plane conditions have been found, the thrust may be calculated. Consider the forces on a stationary motor. The surrounding atmosphere exerts a pressure P_A on all external surfaces and at the nozzle exit plane the pressure is that of the exhaust gas. There is thus a nett forward force on the motor, which is equal to the amount by which the gas pressure at the exit exceeds the

atmospheric pressure, integrated over the nozzle exit plane. The rearward momentum of the gas stream emerging from the nozzle produces a reacting forward force proportional to the momentum flow rate of the gas. Thus the total forward force on the motor, the thrust T , is given by

$$T = 2\pi \int_0^{r_{FIN}} [r\rho u^2 + r(P - P_A)]_{x=x_{FIN}} dr .$$

5 USE OF THE PROGRAMS

The three computer programs are interdependent and, with the exception of ODN0Z, which may be used separately to generate one-dimensional equilibrium exit plane conditions, must be used in the sequence shown in Fig. 1. They are relatively simple to use, requiring only specification of the propellant composition, pressure and enthalpy, nozzle geometry, thermodynamic data and the chemical reaction scheme with rate coefficients. The thermodynamic data and reaction rate coefficients are input via the standard data files THERMDATA and REACTIONS, which are searched by the programs to find the thermodynamic data for the given species and the rate coefficients for the given reactions.

The nozzle geometry may be one of two types, featuring either a conical exit section (Fig. 5a) or a contoured exit section (Fig. 5b). If the nozzle is contoured a least-squares approximation is made to a set of given data points on the nozzle wall (x_i, r_i) , with weights w_i , $i=1,2, \dots, m$, by the method of cubic splines. A cubic spline consists of a set of cubic polynomial arcs joined end to end with continuity in value and in first and second derivatives at each join (or knot). The positions of the interior knots are chosen by the user. The algorithm for fitting cubic splines to a set of data points is taken from Ref. 9.

If the values of the data points are to be read from graphs, sufficient points should be chosen to represent adequately the behaviour of the curve. If the data points are provided they must be supplemented from a hand drawn curve if there are appreciably less than 20 of them. The shape of the curve gives some guidance on the placing of the interior knots. There should not be too many of these as they can produce unwanted fluctuations. The number of data points must exceed the number of interior knots by at least 4. In general, more knots are needed where the behaviour of the curve is changing rapidly, and less where it is changing slowly. The exact positioning of the knots is not critical.

As the program ODNOZ calculates the axial position x from the area A (when performing the throat calculation) and finds A from x at stations downstream of the throat, two cubic spline functions $r = s_x(x)$ and $x = s_r(r)$ must be fitted to the set of data points and hence two sets of knots, at given axial locations for the function in x , and at given radial points for the function in r , must be provided.

An example of a contoured nozzle, providing guidance on the placing of interior knots, is given in Section 6.

ODNOZ and TRANOZ each occupy about 30 K words of store (decimal) and SUPERNOZ requires 40 K. Typical run times for the programs on an ICL 1904S computer are one minute for ODNOZ and two minutes for TRANOZ. The time taken to run SUPERNOZ with no chemical reactions (frozen chemistry) is about one minute, but when chemical reactions are included the time varies considerably, depending on the number of species and reactions. A typical run time is probably about one hour.

5.1 ODNOZ

ODNOZ has two input channels (5 and 7) and two output channels (6 and 9). Channel 5 is used to input the basic data and channel 7 is used to input THERMDATA. Channel 6 produces the general (lineprinter) output, comprising chamber and throat conditions, the solution at a specified number of axial stations downstream of the throat and the equilibrium exit plane conditions. Channel 9 produces the table of flow properties, starting at the throat ($M=1$), required for input to TRANOZ. Care must be taken to ensure that the range of Mach numbers in the table spans the value likely to be encountered at the nozzle throat wall point. This could range from slightly greater than unity for a nozzle with a large normalised throat wall radius of curvature ($R^*/r^* > 3$, say), to about 1.3 for a nozzle with a small normalised throat wall radius of curvature ($R^*/r^* = 0.5$, say).

INPUT CHANNEL 5

Input
No.

- | | | |
|---|--------------------------|---|
| 1 | FORMAT (12A6)
IHEAD : | run title. |
| 2 | FORMAT (510)
IAX : | number of axial stations at which the solution is required to construct the table of flow properties for input to TRANOZ (max. 20). |

Input
No.

ICONT	:	0 for conical nozzle, 1 for contoured nozzle.
ISTOT	:	total number of chemical species (max. 40).
IC	:	number of fundamental species excluding those to be considered chemically inert.
INERT	:	number of inert species.
3	FORMAT (12E0.0)	
TOD	:	initial guess at chamber temperature, K.
POD	:	chamber pressure, atmospheres.
HIN	:	specific enthalpy of the propellant, cal g ⁻¹ .
RL	:	throat radius, cm.
XSTART	:	starting point, downstream of the throat, at which the solution is required for construction of the table of flow properties (usually 0.02 r*), cm.
XFIN	:	distance from throat to nozzle exit plane, cm.
XINC	:	x increment between points in the table of flow properties (usually 0.02 r*), cm.
ACC	:	accuracy, usually 1.0 E-06.

NOZZLE GEOMETRY (see Figs 5a and 5b)

4	FORMAT (12E0.0)	
TH1	:	first inlet cone half angle, deg.
XX1	:	distance from throat (-ve) at which first and second inlet cones meet, cm.
TH2	:	second inlet cone half angle, deg.
X2	:	distance from throat (-ve) at which second inlet cone meets first circular arc throat section, cm.
RAD1	:	first circular arc radius, cm.
X3	:	distance from throat at which first and second circular arcs meet, cm. (+ve, -ve or zero).

Input 5 is included only if the nozzle has a conical exit (ICONT = 0).

Input
No.

5 FORMAT (12E0.0)

RAD2 : second circular arc radius, cm.

X4 : distance from throat to end of second circular arc section, cm.

TH3 : first exit cone half angle, deg.

X5 : distance from throat at which the first and second exit cones meet, cm.

TH4 : second exit cone half angle, deg.

Input group 6 is included only if the nozzle has a contoured exit (ICONT = 1).

6.1 FORMAT (510)

NP : number of data points (max. 40).

NKX : number of intervals (= number of interior knots + 1) for the cubic spline approximation $r = s_x(x)$ (max. 8).

NKR : number of intervals for the cubic spline approximation $x = s_r(r)$ (max. 8).

6.2 FORMAT (12E0.0)

There now follow NP records containing the set of data points (x_i, r_i) with weights w_i .

XC(I) : axial co-ordinate of the ith data point, cm.

Q(I) : radial co-ordinate of the ith data point, cm.

WT(I) : weight of the ith data point (usually $w_i = 1.0$, but if the curve is required to pass exactly through a particular point, e.g. throat or exit plane, set $w_i > 1.0$).

for I=1,2, ... , NP

6.3 FORMAT (12E0.0)

The next record contains the NKX-1 internal knots for fitting the spline function $r = s_x(x)$.

RKX(5) : axial position of the first internal knot, cm.

 :

RKX(J) : axial position of the ith internal knot, cm.

 :

RKX(NKX+3): axial position at the last internal knot, cm.

Input
No.

Eight additional knots are inserted by the program, the first four are set equal to x_1 , the last four to x_{np} .

6.4 FORMAT (12E0.0)

The next record contains the NKR-1 internal knots for fitting the spline function $x = s_r(r)$.

RKR(5) : radial position of the first internal knot, cm.
 ⋮
 RKR(J) : radial position of the jth internal knot, cm.
 ⋮
 RKR(NKR+3) : radial position of the last internal knot, cm.

Eight additional knots are inserted by the program; the first four are set equal to r_1 , the last four to r_{np} .

Input group 7 contains the chemical data.

7.1 FORMAT (A6,E12.6)

There now follow IC records containing the names and concentrations of the fundamental species, and INERT records containing the names and concentrations of the inert species.

IATIT(I) : name of the ith fundamental species.
 Q(I) : number of gram atoms of the ith fundamental species/100 grams of propellant.
 I=1,2, ..., IC
 IATIT(I) : name of the ith (inert) species.
 Q(I) : number of gram atoms of the ith (inert) species/100 grams of propellant.
 I=IC+1, ..., IC + INERT

7.2 FORMAT(A6,18F4.1)

The remaining ISTOT-IC-INERT records contain the names of the dependent species, along with the matrix Λ , which describes the formation of the ith species in terms of the jth fundamental species.

UNLIMITED

IATIT(I) : name of the ith (dependent) species.
ALPHA(I,1): number of moles of the first independent
 : species per mole of the ith species.
 :
ALPHA(I,J): number of moles of the jth independent species
 : per mole of the ith species.
 :
ALPHA(I,IC): number of moles of the last independent
 : species per mole of the ith species.

for I=IC+INERT+1, ISTOT

INPUT CHANNEL 7

Thermodynamic data for chemical species likely to be required in a rocket nozzle calculation are stored in a standard data file, in blocks of 4 records in the form specified in Ref. 10. The thermodynamic data for the species in the calculation are selected by comparing the 6 character name of the first block in the standard data file with each of the species names previously specified. If there is no match the block of data is discarded and the process is repeated with the next block until the thermodynamic data for all the species present in the calculation have been found. If the calculation includes a species not appearing in the standard thermodynamic data file, or if the name is different, the message

"(species name) not in thermodynamic data file"

is output and the calculation is terminated.

The required thermodynamic data are input in the form:

Input
No.

1 FORMAT(A6)

IN : name of species in standard thermodynamic
 : data file.

The following records are saved only if IN=IATIT(J) .

2 FORMAT(4E16.8)

WT(J) : molecular weight of jth species.

AC(9,J) : coefficient a_4 in polynomial expression¹⁰

Input
No.

$$CP(J) = \sum_{n=-4}^4 a_{nj} T^n$$

for specific heat of jth species (cal mol⁻¹ K⁻⁴).

- CS(J) : thermodynamic property C_S (cal mol⁻¹ K⁻¹)¹⁰.
- CH(J) : thermodynamic property C_H (cal mol⁻¹ K⁻¹)¹⁰.
- 3 FORMAT(4E16.8)
- AC(I,J) : coefficients a_{-4} to a_{-1} in polynomial
I=1,4 expression for specific heat of jth species
(cal mol⁻¹ K⁻ⁿ).
- 4 FORMAT(4E16.8)
- AC(I,J) : coefficient a_0 to a_3 in polynomial
I=5,8 expression for specific heat of jth species
(cal mol⁻¹ K⁻ⁿ).

5.2 TRANOZ

TRANOZ has two input channels (1 and 3) and two output channels (2 and 4). Channel 1 is used to input the data defining the transonic flow field and the axial location of the point on the nozzle wall from which the initial data line is constructed for starting the method of characteristics solution (see Fig. 2). The point chosen to start the supersonic solution is usually the throat wall point since the Mach number here is always greater than unity for particle-free flow, and this choice permits a finite rate chemical treatment as far upstream as possible. The transonic flow domain must be large enough to contain the whole of the constant Mach number method of characteristics starting line, but must not extend too far downstream because for large Mach numbers the solution procedure becomes highly unstable and requires a very small relaxation factor, and hence many iterations, to obtain convergence. If the upstream and downstream boundaries are placed at $x = -0.6 r^*$ and $x = 0.8 r^*$ respectively, both these requirements should be satisfied for all nozzles likely to be encountered, with gas phase flow. A relaxation factor of 0.3 is optimum for this configuration, convergence being achieved in all cases in far fewer than 100 iterations. The maximum number of iterations to be permitted in the

calculation and the interval between iterations at which the solution is to be printed are also input.

Channel 3 is used to input the data prepared by ODNOZ. Channel 2 outputs the whole transonic flow field solution, giving either the final solution only, or including the solution at intermediate iterations if required. If the iterative process does not converge to the required accuracy, the message

"maximum number of iterations reached"

is output and the solution at that stage is given. The calculation may also be terminated with the message

"no solution to mass flux equation at $x =$ "

which means that the calculated mass flux at a station just downstream of the throat is less than the required mass flux. This may happen with nozzles which have a very small normalised throat wall radius of curvature ($R^*/r^* < 1$), since in the first iteration the streamline minima are assumed to be at the throat, and for such nozzles they are often well downstream of the throat. Hence, at an axial station just downstream of the throat, some of the streamlines may have negative gradients rather than positive ones, thus causing a large error in the mass flux integration. For this reason the axial step size is always increased to $0.2 r^*$ if the user sets it to less than that. The program may be restarted by increasing the nozzle step size to slightly greater than $0.2 r^*$, to by-pass the region where the streamlines are still converging.

Channel 4 produces the data required for input to SUPERNOZ, comprising chamber conditions, thermochemical data and the properties along the constant Mach number line. A check must be made to ensure that the Mach number at the point on the nozzle wall chosen to start the supersonic solution is contained within the table produced by ODNOZ. Care must also be taken to ensure that the whole of the constant Mach number line lies within the calculated transonic domain. For nozzles with a small normalised throat wall radius of curvature the point where the line crosses the axis can be well downstream of the point where it crosses the wall (see, for example, Fig. 2).

INPUT CHANNEL 1

Input
No.

- 1 FORMAT(100E0.0)
- XSTART : point on nozzle wall from which the initial
 data line is constructed for starting the
 supersonic solution (usually 0.0), cm.
- XSTEP : x increment between axial stations in
 transonic flow field (usually 0.2 r*, if
 xstep < 0.2 r* , program sets xstep =
 0.2 r*), cm.
- XMIN : minimum value of x in transonic flow field
 (usually -0.6 r*), cm.
- XMAX : maximum value of x in transonic flow field
 (usually 0.8 r*), cm.
- RF : relaxation factor (usually 0.3).
- ACC : accuracy, used to test the convergence of the
 Mach number, usually 1.0 E-05.
- 2 FORMAT(310)
- NN : number of radial points in the transonic and
 supersonic flow fields (maximum 16).
- ITER : maximum number of iterations to be permitted
 in the calculation.
- IPRINT : number of iterations between print stations.

5.3 SUPERNOZ

SUPERNOZ has three input channels (1, 5 and 7) and two output channels (2 and 4). Channel 1 is used to input the data produced by TRANOZ, channel 5 is used to input the number of chemical reactions and the name of each reaction as it appears in the standard reaction data file REACTIONS, and channel 7 is used to input the standard reaction data file, containing the reaction mechanisms and rate coefficients of most reactions likely to be significant inside rocket nozzles¹¹. The standard file is searched by the program to find those reactions to be included in the calculation.

Channel 2 produces the general output, comprising the non-equilibrium solution along each data line in the flow (see Fig. 4) and the non-equilibrium, two-dimensional exit plane conditions. Channel 4 outputs the exit plane

conditions for use in preparing the input to a rocket exhaust plume structure program, such as REP¹ or BAFL².

INPUT CHANNEL 5

Input
No.

1 FORMAT(10)

NR : total number of chemical reactions to be
 included in the calculation (max 40).

If NR=0 the gas composition is frozen, and no reaction data are required.

2 FORMAT(13A6)

NUMR(I) : number of reaction (e.g. A1, A2, ...)
 as it appears in the standard reaction data
 file and in Ref. 11.

I=1,NR

INPUT CHANNEL 7

The standard reaction data file REACTIONS contains all the reactions, with rate coefficients, which are listed in Ref. 11. An example of a reaction mechanism with rate coefficients is given in Table 2. The reaction data are input as

FORMAT (A6,2X,6(A6,1X), 1X, E8.2, F4.1, F9.1, 3X, 12)

NUM : number of reaction (e.g. A1,A2, ... etc.)¹¹.

NAME(J) : names of first, second and third
 species on the left side of the reaction.

J=1,3

NAME(J) : names of first, second and third
 species on the right side of the reaction.

J=4,6

AC1 : pre-exponential function B in the reaction
 rate expression $k_f = B \cdot T^a \exp(E/T)$
 (molecule-cm-g units).

AC2 : the exponent a in the above reaction rate
 expression (dimensionless).

AC3 : the Arrhenius factor E in the above
 expression (K).

N1 : 1 for two-body reaction, 2 for three-body
 reaction.

If NUM is not one of the reactions to be included in the calculation, the data are discarded and the next entry in the standard reaction data file is input. However, if NUM = NUMR(I), the names of the species on the left and right hand sides of the reaction equation are compared with the names of the species in the calculation and the stoichiometric coefficients v_{ij} and v'_{ij} of species j in the reaction i on the reactants and products sides respectively, are set to 1 or zero accordingly. The reaction rate coefficient data are saved as

$$K1(I) = AC1 \times 6_{10}^{-23} \text{ if } N1 = 1 \text{ or}$$

$$K1(I) = AC1 \times 6_{10}^{-23} \times 6_{10}^{-23} \text{ if } N1 = 2 \text{ ,}$$

$$K2(I) = AC2 \text{ and } K3(I) = AC3 \text{ .}$$

Then

$$k_{fi} = K1 T^{K2} \exp(K3/T) \text{ cc mol}^{-1} \text{ sec}^{-1} \text{ or } \text{cc}^2 \text{ mol}^{-2} \text{ sec}^{-1} \text{ .}$$

If any of the reactions to be included in the calculation cannot be found in the reaction data file, the message

"(reaction) not found in reaction file"

is output and the calculation is terminated.

6 SAMPLE CALCULATION

A sample calculation was carried out to find the two-dimensional, non-equilibrium exit plane conditions of a liquid bipropellant engine. Table 1 contains the propellant composition and chamber pressure, Table 2 lists the chemical reactions used in the supersonic calculation, and the nozzle geometry is shown in Fig. 6a. The nozzle has a contoured exit section, along which a table of (x, r) values are given. The data points, and the selected axial and radial knots, are shown in Fig. 6b. The input data for the program ODN0Z, which include the names and concentrations of the fundamental species and the names and composition (in terms of the fundamental species) of the dependent species to be included in the calculation are shown in Fig. 7. A typical output station, showing the one-dimensional equilibrium throat conditions, is given in Fig. 8. The transonic flow field, with contours of constant Mach number, is shown in Fig. 9. The nozzle of the test case engine has a normalised throat wall radius of curvature of 1.38, which is relatively small, but the constant Mach number line emanating from the throat wall point ($M = 1.17$), chosen to start the method

of characteristics solution, is shown in Fig. 9 to lie well within the transonic solution domain.

The two-dimensional exit plane profiles of pressure and temperature produced by SUPERNOZ are shown in Figs 10 and 11 respectively, compared with the one-dimensional results from FIRAC³. The value of a two-dimensional treatment is immediately apparent. The one-dimensional program calculates the exit plane pressure to be constant at $0.86_{10} \text{ } 5 \text{ Nm}^{-2}$, whereas SUPERNOZ calculates it to lie between $0.45_{10} \text{ } 5 \text{ Nm}^{-2}$ on the nozzle axis and $2.15_{10} \text{ } 5 \text{ Nm}^{-2}$ on the wall. Similarly, the one-dimensional exit plane temperature is constant at 1790 K whilst that from the two-dimensional program varies between 1680 K and 2250 K.

The variations of the gas properties along the nozzle axis and wall are illustrated in Figs 12 to 14. Fig. 12 shows the axis and wall distribution of pressure. The axis pressure drops at a fairly constant rate throughout the nozzle, whereas the wall pressure falls initially very rapidly in the convergent part of the nozzle and then much more slowly in the expansion region until, when the compression corner is reached, it begins to increase. Similar fluctuation is exhibited by the temperature, as shown in Fig. 13. The variation of the gas velocity along the nozzle is shown in Fig. 14, from which it can also be seen that the exit velocity varies between 2845 ms^{-1} on the axis and 2415 ms^{-1} on the wall.

The engine thrust calculated by the two-dimensional program is not very different from that calculated with the one-dimensional program. SUPERNOZ computed the thrust to be 2110 N, whilst FIRAC³ gave it as 2090 N. However, the exhaust plume of the test case engine calculated by the REP program¹ with two-dimensional nozzle exit plane conditions as input differs significantly from that calculated with uniform exit plane conditions as input. Fig. 15 shows a comparison of the predicted plume centreline temperature profile for the engine under sea level, static conditions with both uniform and non-uniform nozzle exit plane conditions as input. Downstream of the shock region the temperature profiles are similar, but close to the nozzle exit plane they are very different. Although the number and locations of shock waves calculated by the program with the two different sets of inlet conditions are the same, the strengths of the shocks calculated with the two-dimensional exit plane conditions as input are much greater. This could be quite significant in a number of contexts, particularly in a fusing context, where accurate knowledge of the strengths and locations of temperature discontinuities is very important.

7 CONCLUSIONS

A set of computer programs has been written to calculate the two-dimensional flow conditions in axisymmetric nozzles. The chemical species are assumed to be in equilibrium in the combustion chamber and as far as the nozzle throat, whilst frozen or finite rate chemistry may be applied in the supersonic region of the nozzle. A summary of the theoretical basis of the programs is included, with full operating instructions. A sample calculation is presented, illustrating the wide radial variation in rocket exhaust properties which may occur at the nozzle exit plane.

Although the programs do not produce a significant improvement over previous methods³ in accuracy of thrust calculations, they provide far more realistic estimates of nozzle exit plane properties and hence better starting conditions for an exhaust plume structure analysis program^{1,2}. They are particularly important in helping to provide accurate predictions of the shock structure of a rocket exhaust plume.

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TABLE 1Test case parametersFuel

Mono-methyl hydrazine

Oxidant

Dinitrogen tetroxide



Oxidiser/fuel ratio

1.8

Chamber pressure

3.45 MPa (34 atm)

Nozzle throat radius

1.139 cm

Nozzle throat radius of curvature

1.575 cm

 R^*/r^*

1.38

Nozzle exit radius

2.808 cm

TABLE 2

Reaction mechanism for test case

<u>No.</u> ¹¹	<u>Reaction</u>	<u>Rate coefficient</u> ^a	<u>Uncertainty</u> ^b <u>factor</u>
A1	$O + O + M \rightarrow O_2 + M$	$3 \times 10^{-34} \exp(900/T)$	10
A2	$O + H + M \rightarrow OH + M$	$1 \times 10^{-29} T^{-1}$	30
A3	$H + H + M \rightarrow H_2 + M$	$3 \times 10^{-30} T^{-1}$	30
A4	$H + OH + M \rightarrow H_2O + M$	$2 \times 10^{-25} T^{-2}$	10
A5	$CO + O + M \rightarrow CO_2 + M$	$7 \times 10^{-33} \exp(-2200/T)$	30
B1	$OH + H_2 \rightarrow H_2O + H$	$3.6 \times 10^{-11} \exp(-2600/T)$	2
B2	$O + H_2 \rightarrow OH + H$	$3.0 \times 10^{-14} T \exp(-4480/T)$	1.5
B3	$H + O_2 \rightarrow OH + O$	$3.7 \times 10^{-10} \exp(-8450/T)$	1.5
B4	$CO + OH \rightarrow CO_2 + H$	$2.8 \times 10^{-17} T^{1.3} \exp(330/T)$	3
B5	$OH + OH \rightarrow H_2O + O$	$1 \times 10^{-11} \exp(-550/T)$	3
P1	$H + O_2 + M \rightarrow HO_2 + M$	$2 \times 10^{-32} \exp(500/T)$	10
P3	$H + HO_2 \rightarrow OH + OH$	$4 \times 10^{-10} \exp(-950/T)$	5
P4	$H + HO_2 \rightarrow H_2 + O_2$	$4 \times 10^{-11} \exp(-350/T)$	5
P5	$H_2 + HO_2 \rightarrow H_2O + OH$	$1 \times 10^{-12} \exp(-9400/T)$	10
P6	$CO + HO_2 \rightarrow CO_2 + OH$	$2.5 \times 10^{-10} \exp(-11900/T)$	10
P7	$O + HO_2 \rightarrow OH + O_2$	$8 \times 10^{-11} \exp(-500/T)$	30
P8	$OH + HO_2 \rightarrow H_2O + O_2$	1×10^{-10}	30
Q1	$CHO + O \rightarrow CO + OH$	$3 \times 10^{-11} \exp(-2500/T)$	100
Q2	$CHO + OH \rightarrow CO + H_2O$	1×10^{-11}	100
Q3	$CO + H + M \rightarrow CHO + M$	$2 \times 10^{-33} \exp(-850/T)$	100
Q4	$CHO + H \rightarrow CO + H_2$	$2 \times 10^{-10} \exp(-2500/T)$	30
U3	$NO + H + M \rightarrow HNO + M$	$1.5 \times 10^{-32} \exp(300/T)$	10
U4	$HNO + H \rightarrow NO + H_2$	8×10^{-12}	10
U5	$HNO + OH \rightarrow NO + H_2O$	6×10^{-11}	5
U6	$N_2 + O \rightarrow NO + N$	$1.3 \times 10^{-10} \exp(-38000/T)$	5
U7	$N + O_2 \rightarrow NO + O$	$1.1 \times 10^{-14} T \exp(-3150/T)$	3

a ml-molecule-second units

b defined as in Ref. 11

Nomenclature

A	nozzle cross-sectional area normalised by the throat area; diabatic heat addition term linking fluid dynamic and relaxation processes
B	energy exchange term linking fluid dynamic and relaxation processes
c	number of independent chemical species; speed of sound, ms^{-1}
c_j	mass fraction of j th species
C_p	specific heat, J kg^{-1}
f_i	derivative with respect to x of γ_i , $\frac{d\gamma_i}{dx}$
F	function defined by equation (4.17)
G	function defined by equation (4.18)
h_j	enthalpy of the j th species, J mol^{-1}
H	total enthalpy, J mol^{-1} ; function defined by equation (4.19)
$k_{f,i}$	forward rate coefficient for the i th reaction, $\text{cc mol}^{-1} \text{s}^{-1}$ or $\text{cc}^2 \text{mol}^{-2} \text{s}^{-1}$
K_p^j	equilibrium constant for the j th species, based on partial pressures
K_i	equilibrium constant of the i th reaction
m	mixture molecular weight, g mol^{-1}
m_j	molecular weight of j th species, g mol^{-1}
M	Mach number
q_j	initial mole fraction of species j
q_j^0	initial number of moles of j th species per unit mass of propellant
P	pressure, Nm^{-2}
P_a	pressure, atmospheres
r	number of chemical reactions; radial co-ordinate, normalised by throat radius
r^*	throat radius, cm
R	universal gas constant, $8.3143 \text{ J K}^{-1} \text{ mol}^{-1}$, $82.056 \text{ cc atm mol}^{-1} \text{ K}^{-1}$
R^*	nozzle throat wall radius of curvature
s	total number of chemical species

s_j^0	entropy of jth species at 1 atmosphere, $\text{cal mol}^{-1} \text{K}^{-1}$
S	mixture entropy, non-dimensional
T	temperature, K
T_n	non-dimensional temperature, $T_n = T/T_0$
u	axial velocity, ms^{-1}
v	radial velocity, ms^{-1}
V	velocity, ms^{-1}
w_j	net species production rate
x	axial distance from nozzle throat, normalised by throat radius
X_j	mole fraction of species j
α	Mach angle, angle between streamline and Mach line characteristics
α_{ij}	number of moles of species j per mole of species i
β_{ij}	difference between the stoichiometric coefficients of the jth species on the product and reactant sides of the ith reaction, $\beta_{ij} = \nu_{ij}' - \nu_{ij}$
β_i	$\sum_{j=1}^s \beta_{ij}$
γ	isentropic exponent
γ_j	concentration of jth species, mol g^{-1}
δ_{ij}	Kronecher delta
ρ	density, kg m^{-3}
θ	streamline angle
μ_j^0	chemical potential of jth species evaluated under standard pressure conditions (1 atmosphere)
ν_{ij}	stoichiometric coefficient of the jth species on the reactant side of reaction i
ν_{ij}'	stoichiometric coefficient of the jth species on the product side of reaction i
ν_i	$\sum_{j=1}^s \nu_{ij}$

ψ stream function

Subscript

o chamber condition

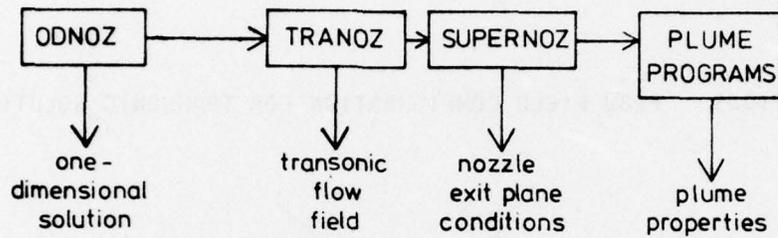
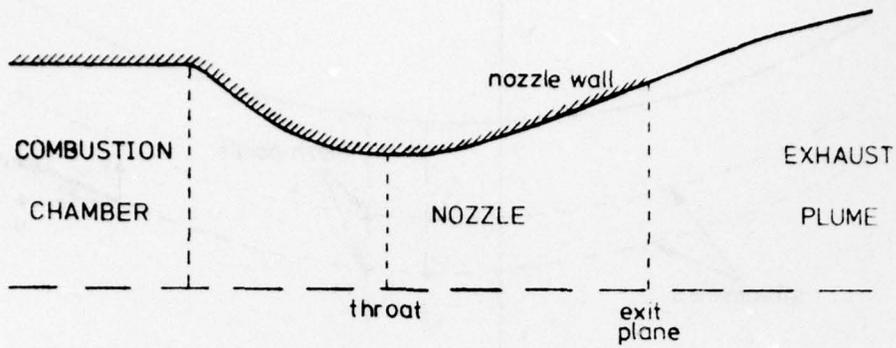


FIG.1 CONVERGENT/DIVERGENT NOZZLE WITH CALCULATION SEQUENCE

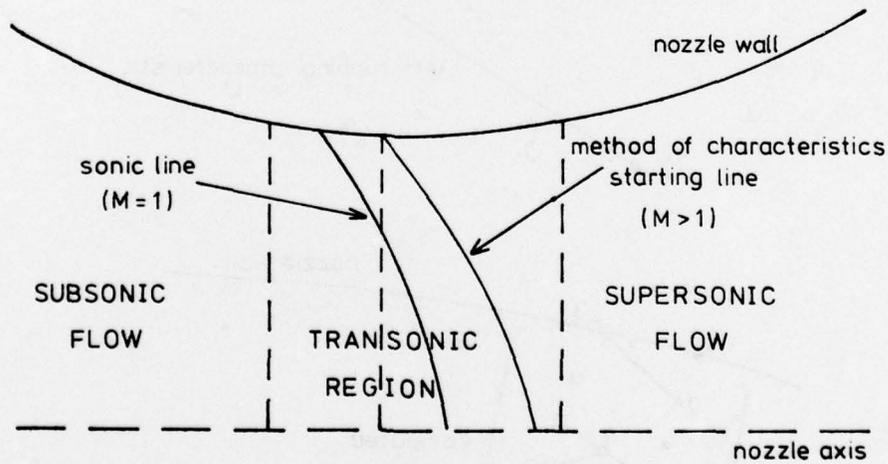


FIG.2 LOCATIONS OF SONIC LINE AND METHOD OF CHARACTERISTICS STARTING LINE

40

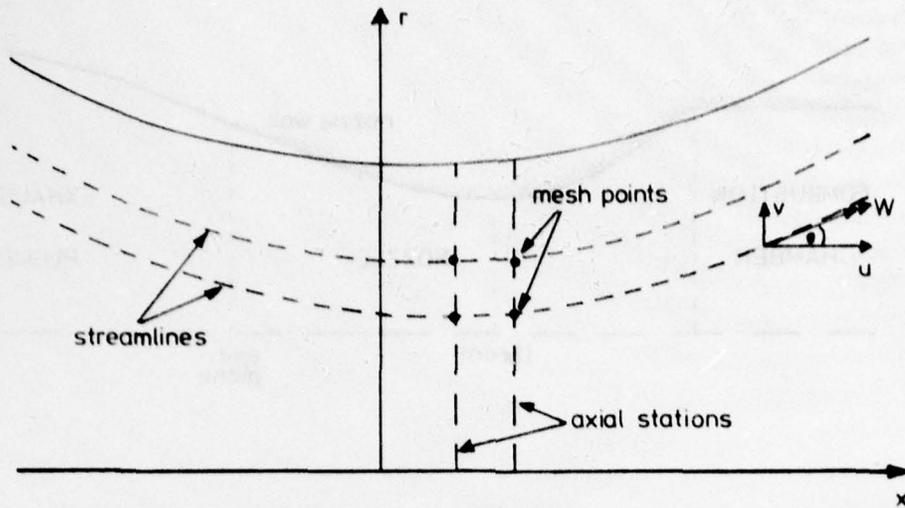


FIG. 3 FLOW FIELD CONFIGURATION FOR TRANSONIC SOLUTION

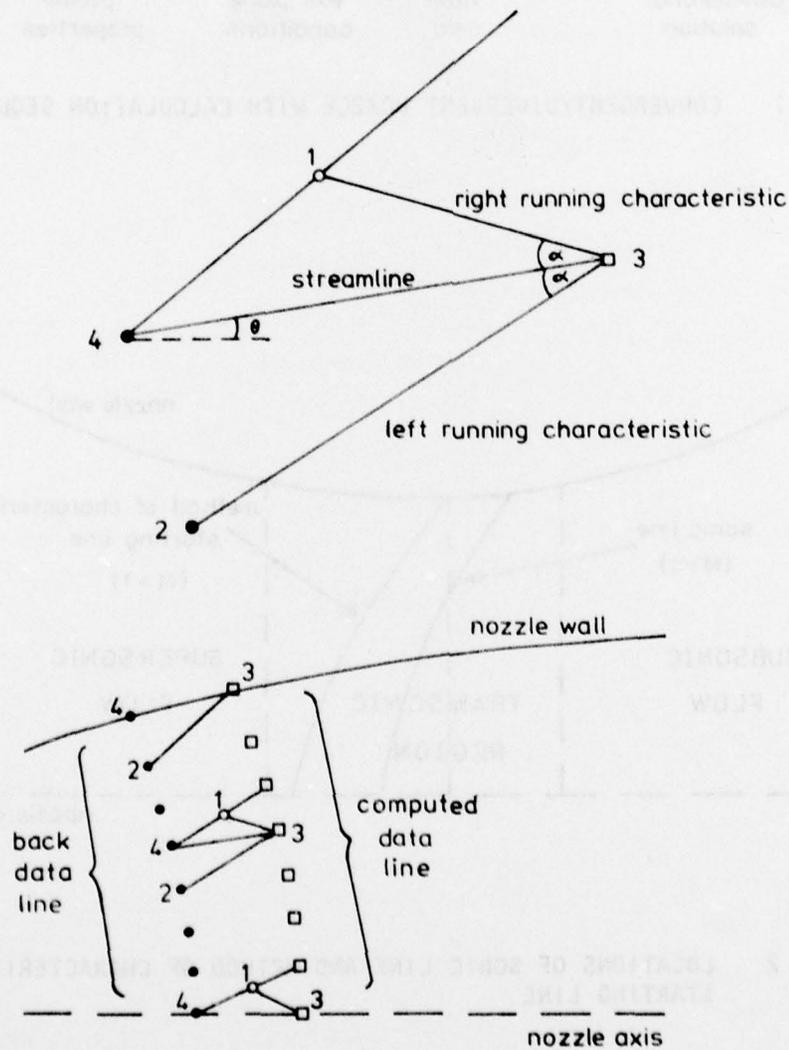


FIG. 4 CHARACTERISTIC MESH FOR SUPERSONIC SOLUTION

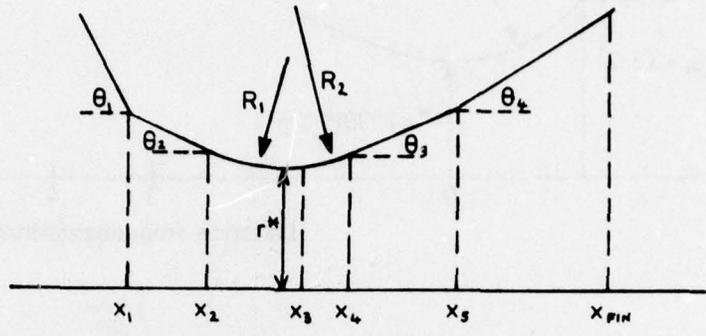


FIG. 5A NOZZLE GEOMETRY - CONICAL EXIT

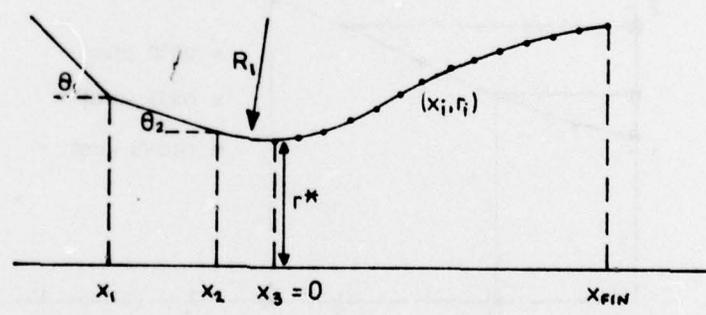


FIG. 5B NOZZLE GEOMETRY - CONTOURED EXIT

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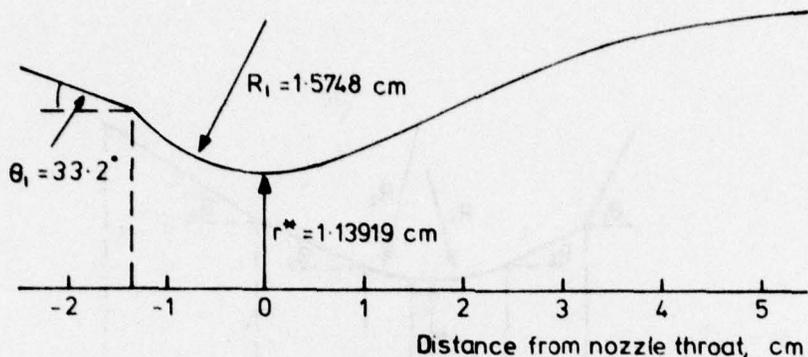


FIG. 6A NOZZLE GEOMETRY OF TEST CASE ENGINE

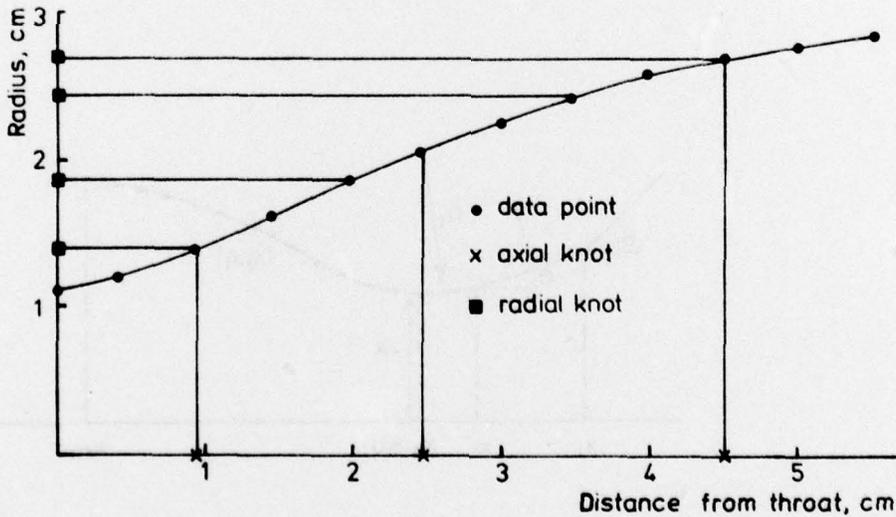


FIG. 6B NOZZLE CONTOUR SHOWING PLACEMENT OF KNOTS

```

TEST CASE
20 1 14 4 0
3200.0 34.0229953 67.8144 1.13919 0.08 5.50672 0.02 1.0E-6
33.233 -1.309144 33.233 -1.309144 1.5748 0.0
12 4 5
0.0      1.13919 5.0
0.42672 1.2065  1.0
0.93472 1.41732 1.0
1.44272 1.65227 1.0
1.95072 1.88468 1.0
2.45872 2.09677 1.0
2.96672 2.28727 1.0
3.47472 2.45237 1.0
3.98272 2.58953 1.0
4.49072 2.69875 1.0
4.99872 2.77495 1.0
5.50672 2.80797 5.0
0.93472 2.45872 4.49072
1.41732 1.88468 2.45237 2.69875
CO      7.750912E-01
H2      2.325273
O2      1.009744
N2      1.473736
CO2     1.0 0.0 0.5 0.0
OH      0.0 0.5 0.5 0.0
H       0.0 0.5 0.0 0.0
O       0.0 0.0 0.5 0.0
HO2     0.0 0.5 1.0 0.0
CHO     1.0 0.5 0.0 0.0
H2O     0.0 1.0 0.5 0.0
N       0.0 0.0 0.0 0.5
NO      0.0 0.0 0.5 0.5
HNO     0.0 0.5 0.5 0.5

```

} CONTOUR DATA

} FUNDAMENTAL SPECIES

} DEPENDENT SPECIES

FIG. 7 INPUT DATA FOR PROGRAM ODNOZ

EQUILIBRIUM THROAT CONDITIONS

TITLE:- TEST CASE

ACCURACY 1.00E-06

	MOLE FRACTION	NO. PER C.C.	
CO	1.182430E-01	5.550612E 18	
H2	1.199625E-01	5.631327E 18	
O2	1.116751E-03	5.242298E 16	
N2	3.156099E-01	1.481549E 19	
CO2	4.833789E-02	2.269097E 18	
OH	1.411050E-02	6.623807E 17	
H	1.321660E-02	6.204190E 17	
O	9.182991E-04	4.310717E 16	
H02	1.852384E-06	8.695536E 13	
CHO	1.689240E-05	7.929700E 14	
H2O	3.661572E-01	1.718830E 19	
N	1.829355E-06	8.587432E 13	
NO	2.305436E-03	1.082227E 17	
HNO	1.471348E-06	6.906862E 13	
TEMPERATURE	3029.93	K	ENTHALPY -8451.1 J MOL-1
MOLECULAR WT.	21.4789	G MOL-1	ENTROPY 11.99101 J MOL-1 K-1
SPECIFIC HEAT	2099.33	J KG-1	
DENSITY	1.67394	KG M-3	VELOCITY 1167.01 M SEC-1
PRESSURE	19.3763	ATM	MACH NO. 1.00730
GAMMA	1.13777		
CSTAR	1741.63	M SEC-1	
MASS FLOW	0.796	KG SEC-1	

FIG. 8 TYPICAL OUTPUT STATION FROM PROGRAM ODNOZ SHOWING ONE-DIMENSIONAL EQUILIBRIUM THROAT CONDITIONS

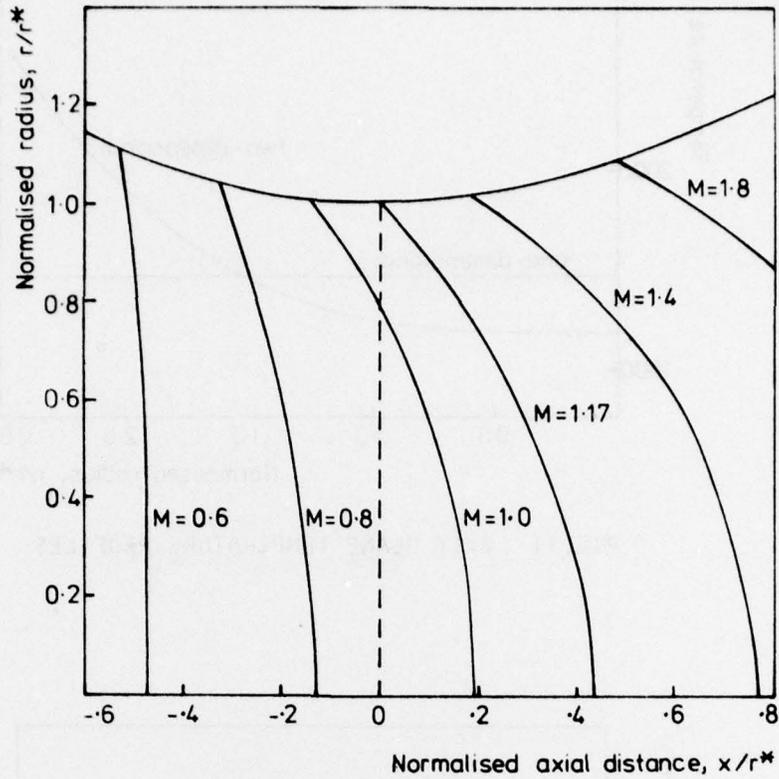


FIG.9 TRANSONIC FLOW FIELD OF TEST CASE ENGINE SHOWING CONTOURS OF CONSTANT MACH NUMBER AND THE METHOD OF CHARACTERISTICS STARTING LINE (M = 1.17)

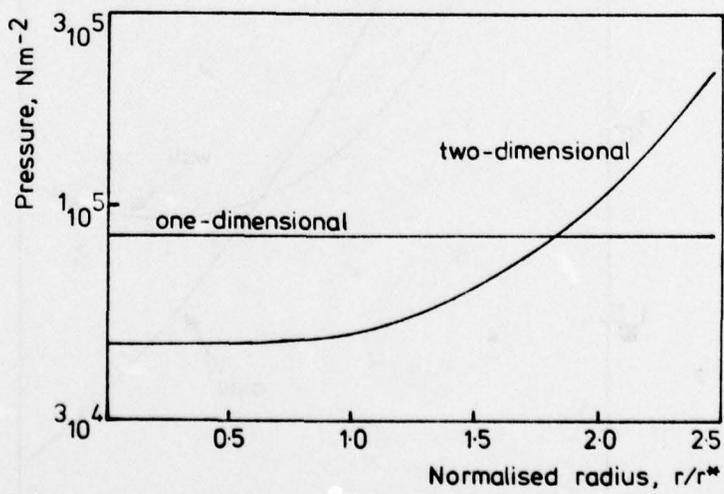


FIG.10 EXIT PLANE PRESSURE PROFILES

9.6

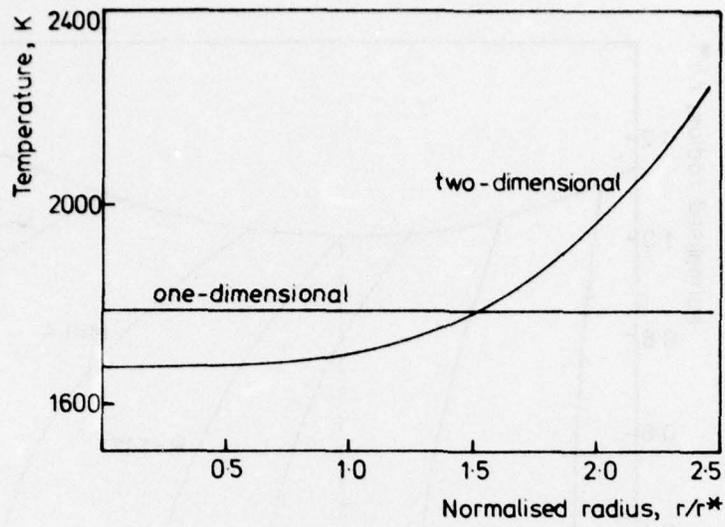


FIG. 11 EXIT PLANE TEMPERATURE PROFILES

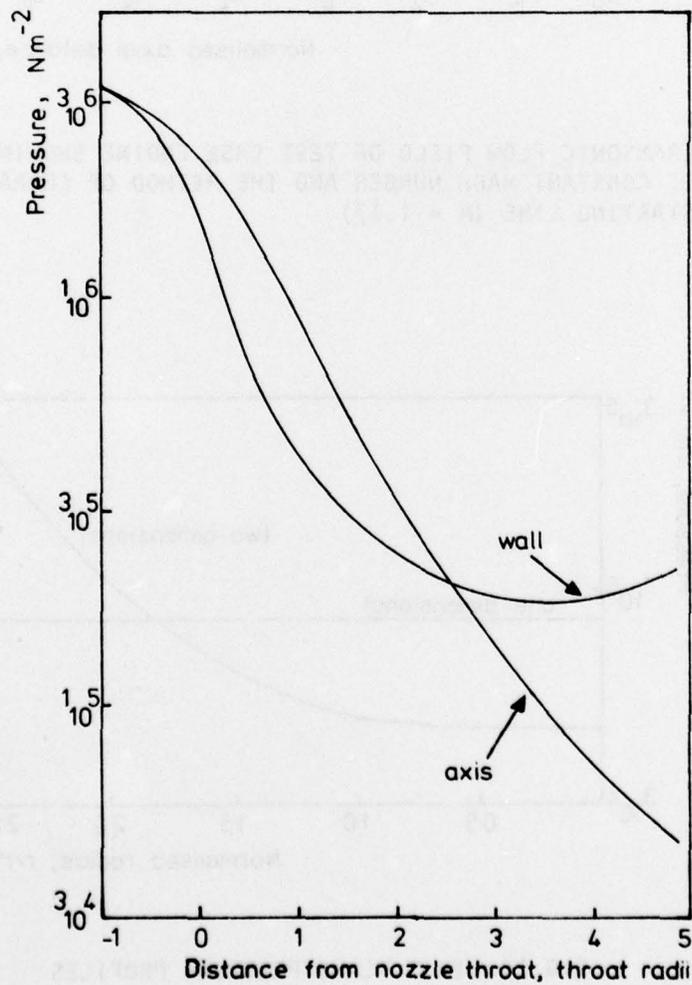


FIG. 12 PRESSURE DISTRIBUTION ALONG NOZZLE

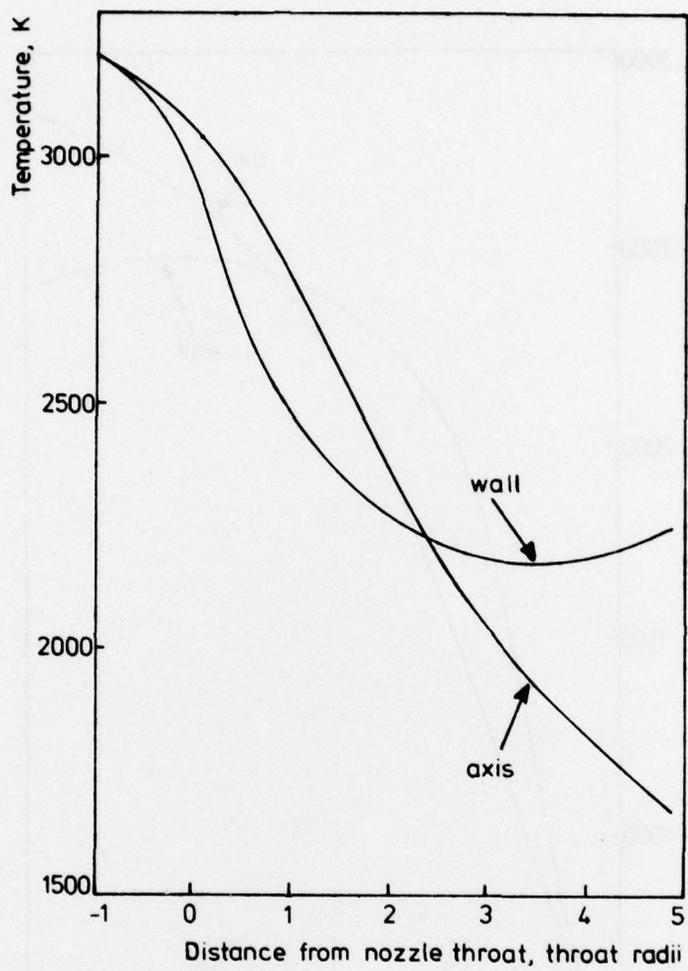


FIG. 13 TEMPERATURE DISTRIBUTION ALONG NOZZLE

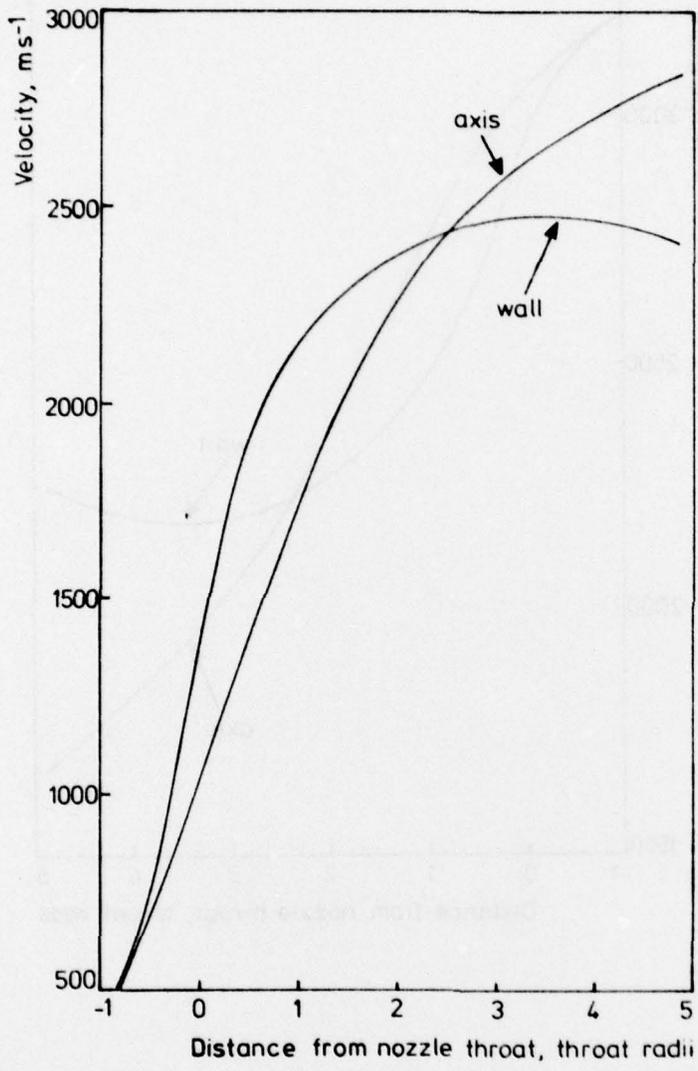


FIG.14 VELOCITY DISTRIBUTION ALONG NOZZLE

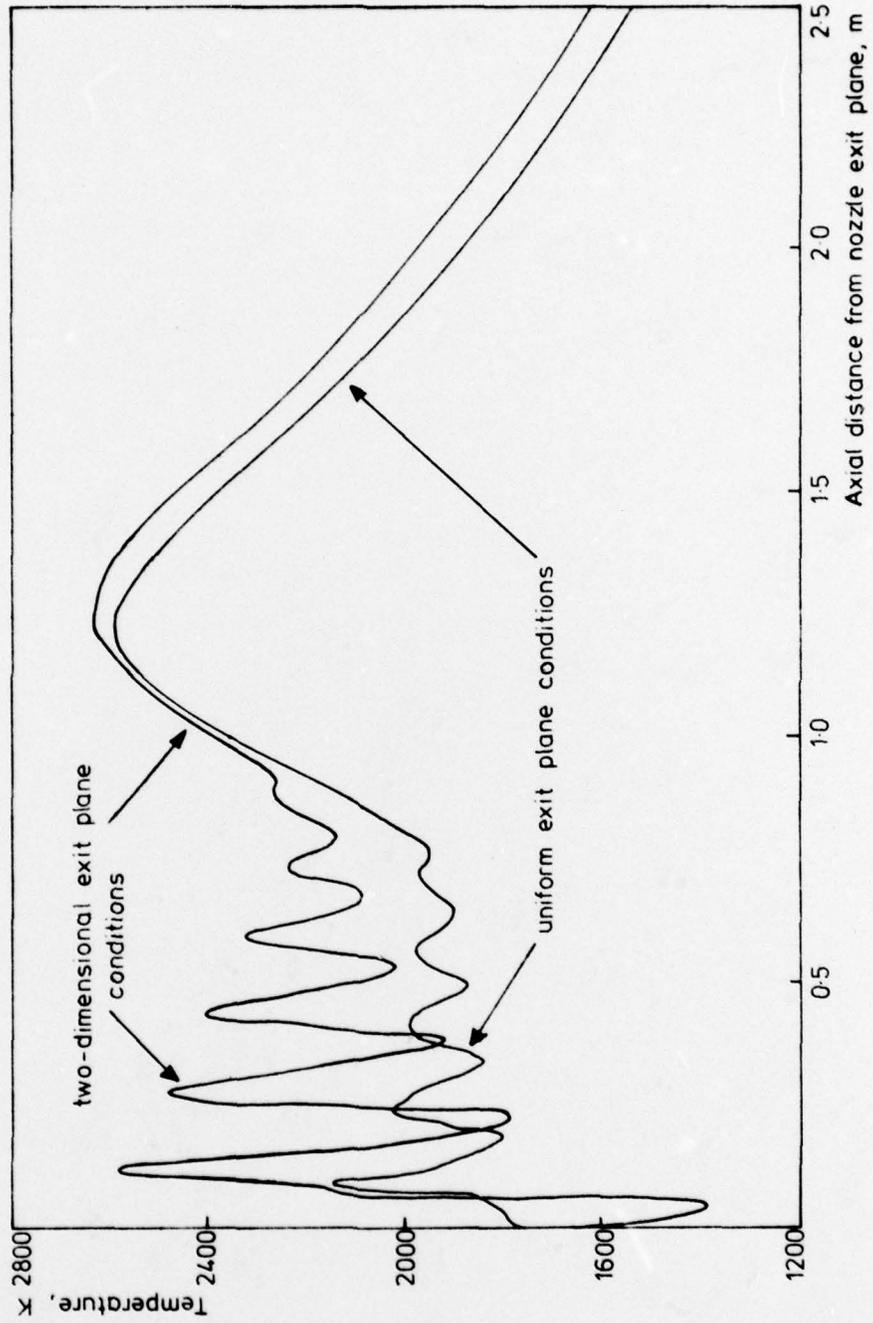


FIG.15 CENTRELINE TEMPERATURE OF EXHAUST PLUME FROM TEST CASE ENGINE. SEA LEVEL, STATIC CONDITIONS

DOCUMENT CONTROL SHEET
(Notes on completion overleaf)

Overall security classification of sheet **UNCLASSIFIED**

(As far as possible this sheet should contain only unclassified information. If it is necessary to enter classified information, the box concerned must be marked to indicate the classification eg (R),(C) or (S)).

1. DRIC Reference (if known)	2. Originator's Reference Technical Report No. 84	3. Agency Reference	4. Report Security Classification Unlimited
5. Originator's Code (if known) 7281500 M	6. Originator (Corporate Author) Name and Location Propellants, Explosives and Rocket Motor Establishment Westcott, Aylesbury, Bucks		
5a. Sponsoring Agency's Code (if known)	6a. Sponsoring Agency (Contract Authority) Name and Location		
7. Title Computer programs to calculate chemically reacting flow in axisymmetric nozzles			
7a. Title in Foreign Language (in the case of translations)			
7b. Presented at (for conference papers). Title, place and date of conference			
8. Author 1, Surname, initials COUSINS, J.M.	9a. Author 2	9b. Authors 3, 4...	10. Date pp ref 5.1978 50 11
11. Contract Number	12. Period	13. Project	14. Other References
15. Distribution statement			
<p style="text-align: center;">Descriptors (or keywords) (TEST)</p> <p>Rocket nozzles; Rocket exhaust; Supersonic flow; Transonic flow; Chemical reactions; Axisymmetric flow; Computer programs</p> <p style="text-align: right;">continue on separate piece of paper if necessary</p>			
<p>Abstract</p> <p>This report describes a set of computer programs which calculates the inviscid two-dimensional expansion of gaseous exhaust mixtures through rocket nozzles. Equilibrium chemistry in the combustion chamber and as far as the nozzle throat is assumed, whilst finite rate or frozen chemistry may be applied from the throat onwards. The transonic flow field is calculated by the method of streamline curvature and the flow in the supersonic region of the nozzle is solved by the method of characteristics.</p> <p>The theory on which the programs are based is summarised and a comprehensive user's guide is included. A sample calculation is presented.</p>			