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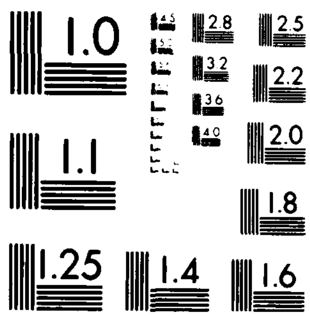
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by

Robert P. Gilbert

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Technical Report No. 48A



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This Technical Report is meant only for internal review, as it would be difficult to imagine the contents are not known to those active in the field. The purpose in writing it is to provide Institute members with a concise discussion on the computation of the flow behind a shock leading to detonation in a one-dimensional system. The computation would be performed using the method of characterisrics, and this reduction would also be ~~utilised~~ used later for our investigation of the stochastic initiation of detonations. Stochastic effects might be introduced either as white noise or as variations in material

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20. Abstract cont.

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# ON THE INITIATION OF DETONATION IN A ONE-DIMENSIONAL SYSTEM

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The present deterministic system is supposed to consist of material whose equation of state resembles that of a polytropic gas. We assume that the system is originally shocked by an infinite piston moving at a constant velocity, and that this shock is sufficient to start certain chemical reactions. These reactions initiate a detonation front (shock wave), which in turn will propagate through the system and sustain the chemical reactions in a zone immediately behind the front. The reaction is assumed to transform undetonated substance into a material with similar thermodynamic properties, plus a certain amount of heat energy. The rate at which heat energy is released depends on the local thermodynamic, and progress variables.

At this point we introduce the notations that are used in this work.

$x$ - distance measured from an original point

$t$ - time measured from the initial point

$u$ - particle velocity

$\rho$ - material density

$\tau$ - specific volume, $\tau = \frac{1}{\rho}$

$S$ - specific entropy

$e$ - specific internal energy

$q$ - heat energy

$i$ - specific enthalpy, $i = e + p\tau$

$c$ - velocity of sound

$p$ - pressure

$T$ - temperature

$\beta$ - adiabatic constant

$C_\tau$ - specific heat at constant specific volume

$U$ - shock velocity

$g$ - $d\beta/dt$

$k_1$, $k_2$, $a_1$, $a_2$, $b_1$, $b_2$, $\rho_o$, $U_A$, $Q$, $\gamma$, are constants

Given Data

$U_A$ - piston velocity

$\rho_o$ - density of unshocked gas

Q - energy of formation of detonation products

$k_1$, $k_2$ - Constants in the rate equation

$a_1$, $a_2$, $b_1$, $b_2$ - constants in the iteration routines

$\gamma$ - equation of state constant

$t_{oo}$,

N, - number of points on each $C^+$ characteristic

We also introduce the following notation for derivatives.

$$A_x := \frac{\partial A}{\partial x}, \; A_t := \frac{\partial A}{\partial t}; \; \dot{A} := \frac{dA}{dt} \equiv \frac{\partial A}{\partial t} + u\frac{\partial A}{\partial x} .$$

1. The Mathematical Model:

In the regions of space-time in which shocks are absent the flow is to be governed by the following conservation equations.

(mass) $\rho_t + u\rho_x + \rho u_x = 0,$ ____________(1.1)

(momentum) $u_t + uu_x + \frac{1}{\rho} p_x = 0,$ ____________(1.2)

(energy) $T\dot{S} = \dot{q} = \dot{e} + p\dot{\tau} .$ ____________(1.3)

Outside of the reaction zone (3) may be replaced by $\dot{S} = 0$; that is the entropy does not change along a particle-path or stream-line. In the reaction zone it is convenient to express the energy balance (1.3) by the following.

$$\dot{q} := Q\dot{\beta} = \dot{e} + p\dot{\tau}, \qquad (1.3')$$

and

$$\dot{\beta} = g(\rho,p,\beta), \qquad (1.4)$$

where $g(\rho,p,\beta)$ is a function of the density, the pressure, and the progress variable $\beta$ which describes the chemical kinetics of the material.

The questions 1.1, 1.2, 1.3', 1.4 are a system of first order partial differential of the form,

$$L_i[\phi] := a_{ij}\frac{\partial\phi^j}{\partial x} + b_{ij}\frac{\partial\phi^j}{\partial t} + c_i = 0, \qquad (1.5)$$

$$(i = 1,2,3,4),\ (j = 1,2,3,4),$$

where the coefficients a, b, c, depend on x, t, $\phi^k$. A necessary and sufficient condition is given for the existence of <u>characteristic directions</u> for this system of equations, that is conditions (for the existence of curves $C_k$, such that a directional derivative $\lambda_i L_i$ may be formed in the same direction as $C_k$. [1], [2] The necessary and sufficient conditions for characteristic direction is that the following homogeneous equations for the $\lambda_i$ be compatible [1], [2]

$$\begin{aligned} &\lambda_i(a_{ij}t_\sigma - b_{ij}x_\sigma) = 0, \\ &\lambda_i(a_{ij}\phi_\sigma{}^j + c_i x_\sigma) = 0, \\ &\lambda_i(b_{ij}\phi_\sigma{}^j + c_i t_\sigma) = 0, \end{aligned} \qquad (1.6)$$

where j = 1,2,3,4. If one sets the determinant of the first four equations

$$|a_{ij}t_\sigma - b_{ij}x_\sigma| = 0,$$

we may obtain an algebraic relation for $\frac{dx}{dt} = \frac{x_\sigma}{t_\sigma}$. By making the following association

$$\phi^1 := \rho,\ \phi^2 := u,\ \phi^3 := p,\ \phi^4 := \beta,$$

and formally computing this determinant one obtains

$$||a_{ij}t_\sigma - b_{ij}x_\sigma|| = \frac{(ut_\sigma - x_\sigma)^2}{\rho(\gamma-1)} \left( [ut_\sigma - x_\sigma]^2 - \gamma t_\sigma{}^2 - \frac{p}{\rho} \right). \qquad (1.7)$$

The characteristics are then given by the equations

$$I_{+,-}: \quad ut_\sigma - x_\sigma = \pm t_\sigma \sqrt{\frac{\gamma p}{\rho}} = \pm t_\sigma c, \qquad (1.8)$$

$$I_0 : \quad (ut_\sigma - x_\sigma)^2 = 0. \qquad (1.9)$$

The first two $I_+$, $I_-$, represent the paths of <u>sound waves</u>, whereas the second two (a double root), $I_0$, are <u>degenerate characteristics</u> and coincide with the <u>streamlines</u>.

The remaining equations in the system (1.6) give rise to <u>compatability conditions</u> on the thermodynamic variables in order that (1.8) and (1.9) be characteristics. Corresponding to the characteristics $I_{+,-}$ we have the compatability conditions,

$$II_{+,-} : \pm\rho u_\sigma + \frac{p_\sigma}{c} = Qg\rho \frac{(\gamma-1)}{c}, \qquad (1.10)$$

and corresponding to $I_0$, we have

$$II_0 : N_\sigma = gt_\sigma. \qquad (1.11)$$

Because the flow is non-adiabatic in the reaction zone ($\dot{S} \neq 0$) one can not introduce Riemann invariants by integrating $II_{+,-}$.

2. <u>On the Numerical Computation of the Characteristics</u>:

In this section we will develop a method by which the characteristics can be approximated. We shall assume that two neighboring points $P_2$, $P_3$ are given on an $I_+$ characteristic, and that $P_1$ lies on the $I_-$ characteristic through $P_2$. Furthermore, the image points* in the (u,p)-plane, $\pi_1$, $\pi_2$, $\pi_3$, will also be assumed known. If the points $P_k$ are sufficiently close the characteristics, which join them may in general be approximated by parabolic arcs. In this case, we may write that on $I_+$, one has

$$\frac{x_4-x_1}{t_4-t_1} \cong \frac{1}{2}\left[\left(\frac{dx}{dt}\right)_4 + \left(\frac{dx}{dt}\right)_1\right] = \frac{1}{2}\left[u_4+c_4+u_1+c_1\right], \qquad (2.1)$$

or by introducing a <u>bar</u> and <u>double subscript</u> for the average value at two positions,

* For each point P $\varepsilon$ (x,t)-plane there corresponds an <u>image point</u>
$\pi$ $\varepsilon$ (u,p)-plane, given by the correspondence u :=u(x,t), p :=p(x,t).

$$I_+ \ : \ \frac{x_4-x_1}{t_4-t_1} \simeq \overline{u_{14}} + \overline{c_{14}} \qquad (2.2)$$

The compatability condition, $II_+$, become

$$\frac{u_4-u_1}{p_4-p_1} \simeq -\left(\overline{\frac{1}{\rho c}}\right)_{14} + 2Q\left(\overline{\frac{g}{c}}\right)_{14}\left(\frac{t_4-t_1}{p_4-p_1}\right) . \qquad (2.3)$$

On $I_-$, and $II_-$ one has respectively

$$\frac{x_4-x_3}{t_4-t_3} \simeq \overline{u_{43}} - \overline{c_{43}} , \qquad (2.4)$$

and

$$\frac{u_4-u_3}{p_4-p_3} \simeq \left(\overline{\frac{1}{\rho c}}\right)_{34} - 2Q\left(\frac{g}{c}\right)_{34}\left(\frac{t_4-t_3}{p_4-p_3}\right) \qquad (2.5)$$

In order to obtain a first estimate of $u_4$, $\rho_4$, $S_4$, we replace the secants $\overline{\pi_4\pi_1}$, $\overline{\pi_4\pi_3}$, by the tangent lines at $\pi_1$ and $\pi_3$, that is by the lines drawn through $\pi_1$ and $\pi_3$ with the respective slopes

$$\left(\frac{du}{dp}\right)_1 = -\left(\frac{1}{\rho c}\right)_1 + 2Q\left(\frac{g}{c}\right)_1 \cdot \left(\frac{dp}{dt}\right)_1^{-1} , \qquad (2.6)$$

and

$$\left(\frac{du}{dp}\right)_3 = \left(\frac{1}{c}\right)_3 - 2Q\left(\frac{g}{c}\right)_1 \cdot \left(\frac{dp}{dt}\right)_1^{-1} . \qquad (2.7)$$

The intersection of the tangent lines yields an estimate for the point $\pi_4$, $\pi_4{}^* = (u_4^*, p_4^*)$, which we use to estimate $\rho_4$, and $c_4$.

If our material is a polytropic gas, then it obeys an equation of state having the form,

$$p = (\gamma-1)\rho^{\gamma} \ \exp\left[\frac{S-S_0}{C}\right] \qquad \text{\_\_\_\_\_\_\_\_(2.8)}$$

where $S_0$ an appropriate constant. Since, we have an estimate for $P_4$, knowledge of either S or $\rho$ at $\pi_4$ implies knowledge of the other. We may obtain an estimate of $S_4$ by making use of the degenerate characteristics, $I_0$, $II_0$. Along $II_0$ we have

$$TS_\alpha = \frac{p}{(\gamma-1)\rho\ C_\tau}\ S_\alpha = Q\beta_\alpha = gt_\alpha, \qquad \text{\_\_\_\_\_\_\_\_(2.9)}$$

or

$$\frac{\rho^{\gamma-1}}{C_v}\ S_\alpha = \exp\left[\frac{S_0-S}{C_\tau}\right]\ gt_\alpha\ . \qquad \text{\_\_\_\_\_\_\_\_(2.10)}$$

We estimate $S_4 \stackrel{\sim}{=} S_4{}^*$ by assuming the streamline passes through $P_1$ and $P_4$, and then

$$\frac{S_4{}^*-S_1}{t_4-t_1} \stackrel{\sim}{=} \frac{C_\tau g_1}{\rho_1^{\gamma-1}} \exp\left[\frac{S_o-S_1}{C_v}\right] \qquad \text{\_\_\_\_\_\_\_\_(2.11)}$$

and which in turn allows us to approximate $\rho_4 \stackrel{\sim}{=} \rho_4{}^*$. An estimate for $c_4$ may be obtained from

$$c_4{}^2 \stackrel{\sim}{=} \left(\frac{\partial p}{\partial \rho}\right)_4^* = \gamma p_4{}^* = \gamma(\gamma-1)(\rho_4{}^*)^{\gamma-1}\exp\left[\frac{S_4{}^*-S_o}{C_v}\right]. \qquad \text{\_\_\_\_\_\_\_\_(2.12)}$$

A point $P_4{}^*$ may be found by computing the ratios $\frac{x_4-x_1}{t_4-t_1}$, $\frac{x_4-x_3}{x_4-t_2}$ from the approximate values $u_4{}^*$, $c_4{}^*$.

We recall, that in order to approximate $S_4$ at $P_4$ we assumed that the streamline passed through $P_1$, $P_4$. To improve this estimate we may compute the slope of $I_0$ at $P_4$, and obtain the intersection of this line with $I_+$ or $I_-$. (See Figure 2). We call the intersection $P_5$, which we estimate by

$$\frac{x_4-x_5}{t_4-t_5} \approxeq \left(\frac{dx}{dt}\right)_4 = u_4 \approxeq u_4^* \qquad (2.13)$$

The value of u, S at $P_5$ may be obtained by interpolation using the values of u, S at $P_1$, $P_2$, $P_3$. The secant of the $I_0$ through $P_4$, $P_5$ then has the slope

$$\frac{x_4-x_5}{t_4-t_5} = \frac{1}{2}(u_4^*+u_5) \ . \qquad (2.14)$$

We may obtain an improved approximation of $S_4$, now using the difference expression,

$$S_4-S_5 \approxeq (t_4-t_5)\ \frac{C_v(\overline{g})_{45}}{\overline{(\rho_{15}^{\gamma-1})}_{45}} \left( \exp\left[\frac{S_0-S}{C_v}\right]\right), \qquad (2.15)$$

where averages are taken from values obtained at $P_5$ and the first estimates at $P_4$. With this value of $S_4$ we can obtain another estimate for $\rho_4$ from the equation of state. Using these new estimates of $\rho_4$, $P_4$, $S_4$ etc. We may now improve our location of $\pi_4$ in the (u,p)-plane by means of the difference formulae for secants instead of the tangent approximation.

If the differences between first and second estimates appears too large, it is suggested that the procedure outlined above be repeated. We include at this point details from the scheme to compute the flow behind the shock, which we assumed is strong. Furthermore, we restrict our investigation to the consideration of reaction rates of the form $g := k_1 \exp\left(\frac{-k_2\rho}{p}\right)$. Our scheme consists of three routines which we lable (A), (B), (C). These are indicated in what follows. We use

(A) for general points,

(B) for piston path points,

(C) for shock points.

We intiate our calculations at point A (See Figure 1), and calculate

$$U_A = \frac{\gamma+1}{2} u_A,\ p_A = \rho_o U_A u_A,\ \rho_A = \frac{\gamma+1}{\gamma-1} \rho_o,\ C_A = \left(\frac{\gamma p_A}{\rho_A}\right)^{1/2},$$

$\beta_A = 0$, and $g_A = k_1\, C^{-k_2 \rho_A / p_A}$. Then let us use the symbol $\vartheta$ to indicate a generic variable, i.e. $\gamma = U, u, p, \rho, c, \beta, g$, and let $\gamma_{oo} = \gamma_A$, $x_{oo} = U_{oo}\, t_{oo}$

Use routine (B) to get the solution at point 10.

(here A=1, oo=2, 10=3)

Use routine (C) to get the solution at point 1N. Divide $C_1^+$ into N parts and interpolate for the values of the variables, i.e.,

$$x_{kj} := x_{10} + \frac{j}{N} (x_{1N} - x_{10})$$

$$\gamma_{ij} := \gamma_{10} + (x_{ij} - x_{10}) \left(\frac{\gamma_{1N} - \gamma_{10}}{x_{1N} - x_{10}}\right), \quad \gamma = t,\ p,\ \rho,\ u,\ c,\ \beta,\ g$$

Calculate 20, 21,.....2N, 30, 31..... 3N, etc.

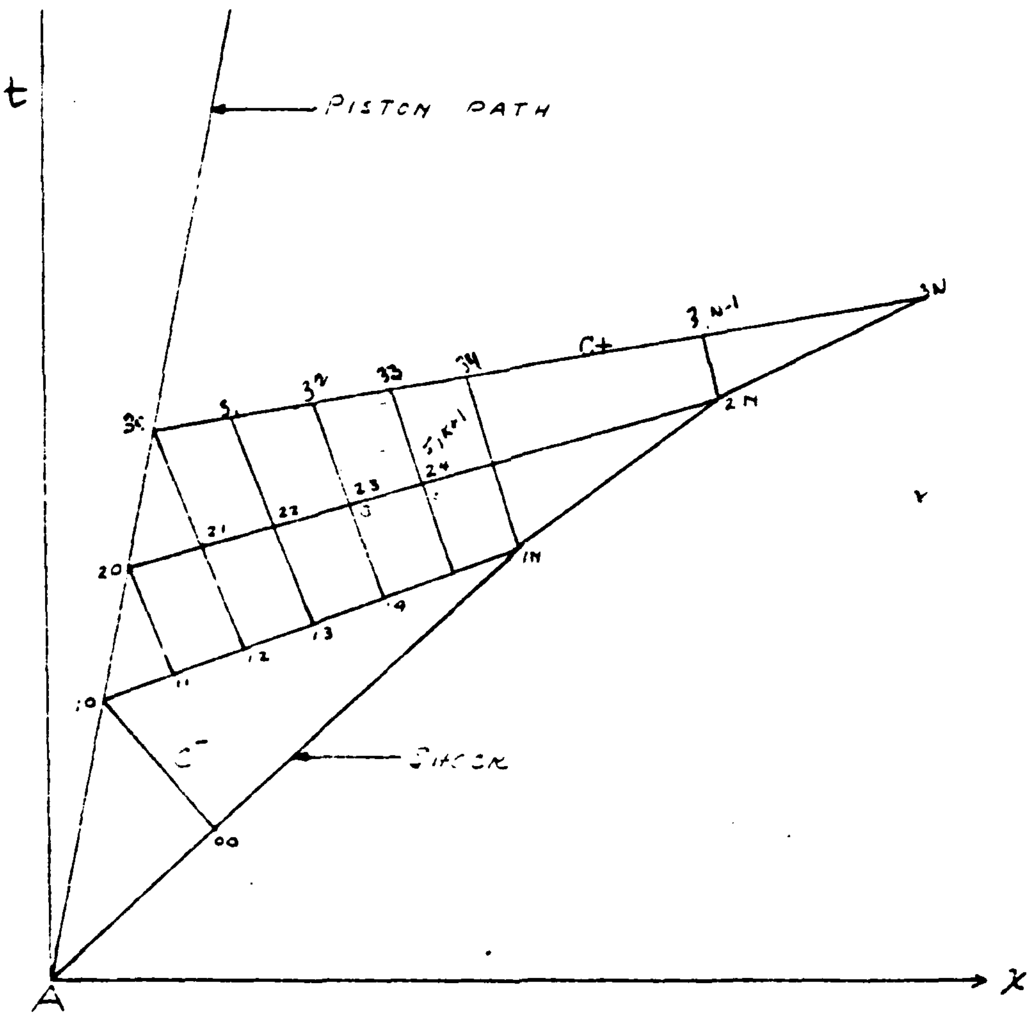



FIGURE 1

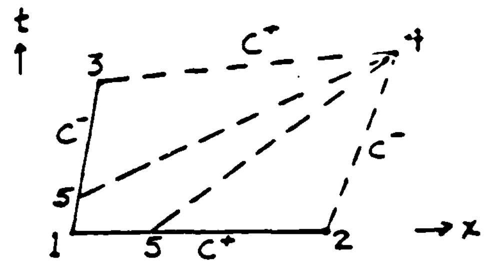
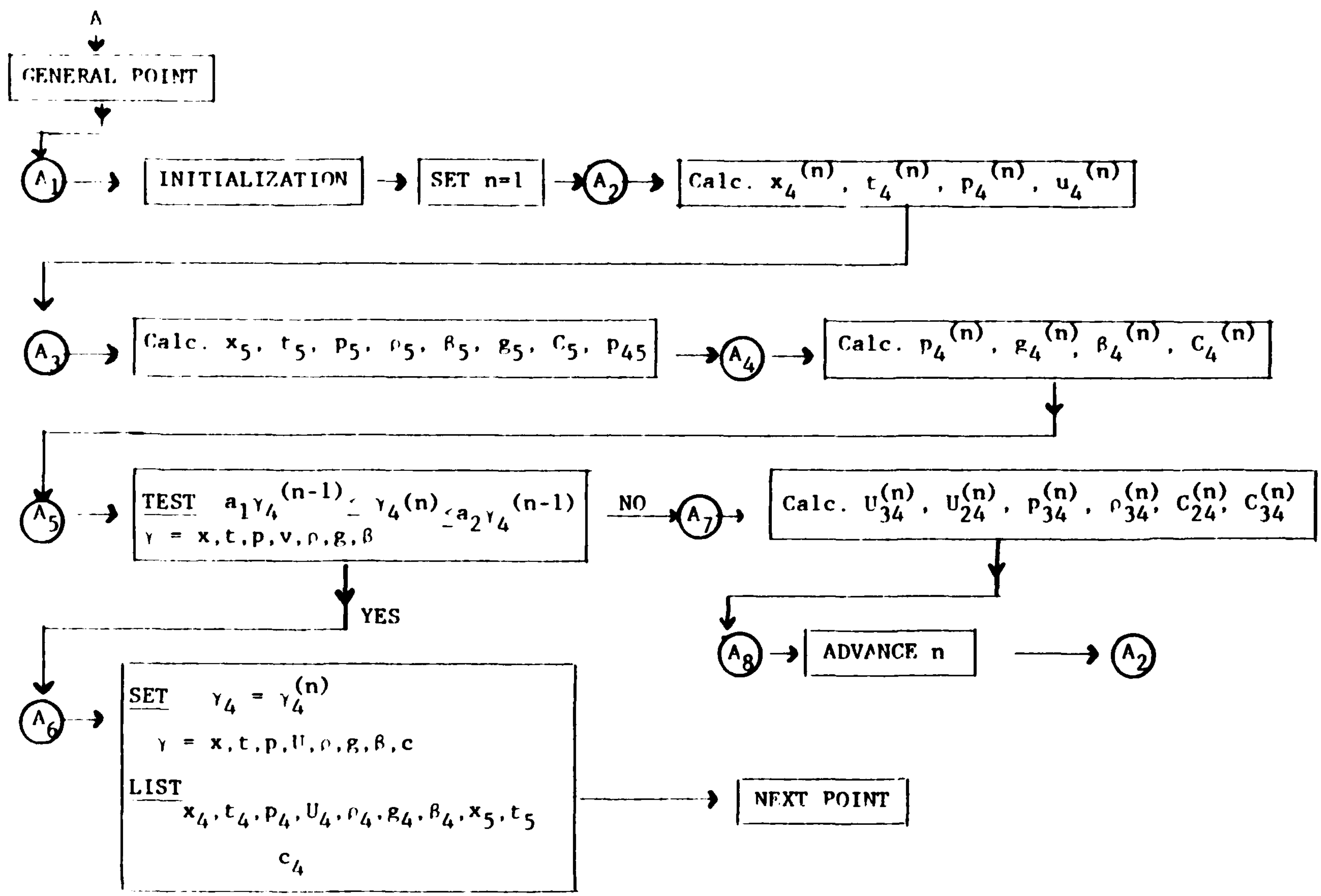



FIGURE 2


A
GENERAL POINT
A1
INITIALIZATION
SET n=1
A2
Calc. $x_4^{(n)}$, $t_4^{(n)}$, $p_4^{(n)}$, $u_4^{(n)}$
A3
Calc. $x_5$, $t_5$, $p_5$, $\rho_5$, $\beta_5$, $g_5$, $C_5$, $p_{45}$
A4
Calc. $p_4^{(n)}$, $g_4^{(n)}$, $\beta_4^{(n)}$, $C_4^{(n)}$
A5
TEST $a_1\gamma_4^{(n-1)} \leq \gamma_4(n) \leq a_2\gamma_4^{(n-1)}$
$\gamma = x,t,p,v,\rho,g,\beta$
NO
A7
Calc. $U_{34}^{(n)}$, $U_{24}^{(n)}$, $p_{34}^{(n)}$, $\rho_{34}^{(n)}$, $C_{24}^{(n)}$, $C_{34}^{(n)}$
YES
A8
ADVANCE n
A2
A6
SET $\gamma_4 = \gamma_4^{(n)}$
$\gamma = x,t,p,U,\rho,g,\beta,c$
LIST $x_4,t_4,p_4,U_4,\rho_4,g_4,\beta_4,x_5,t_5$
$c_4$
NEXT POINT

$A_1 \rightarrow$

**INITIALIZATION**

$U_{34}^{(0)}=U_3,\ U_{24}^{(0)}=U_2,\ C_{34}^{(0)}=C_3,\ C_{24}^{(0)}=C_2,\ P_{34}^{(0)}=P_3,\ \rho_{24}^{(0)}=\rho_2,\ g_{34}^{(0)}=g_3,\ g_{24}^{(0)}=g_2$

$x_4^{(0)}=0,\ t_4^{(0)}=0,\ U_4^{(0)}=0,\ p_4^{(0)}=0,\ \rho_4^{(0)}=0,\ g_4^{(0)}=0,\ \beta_4^{(0)}=0.$

SET n=1

$A_2$

**Calc. $x_4^{(n)},\ t_4^{(n)},\ p_4^{(n)},\ U_4^{(n)}$**

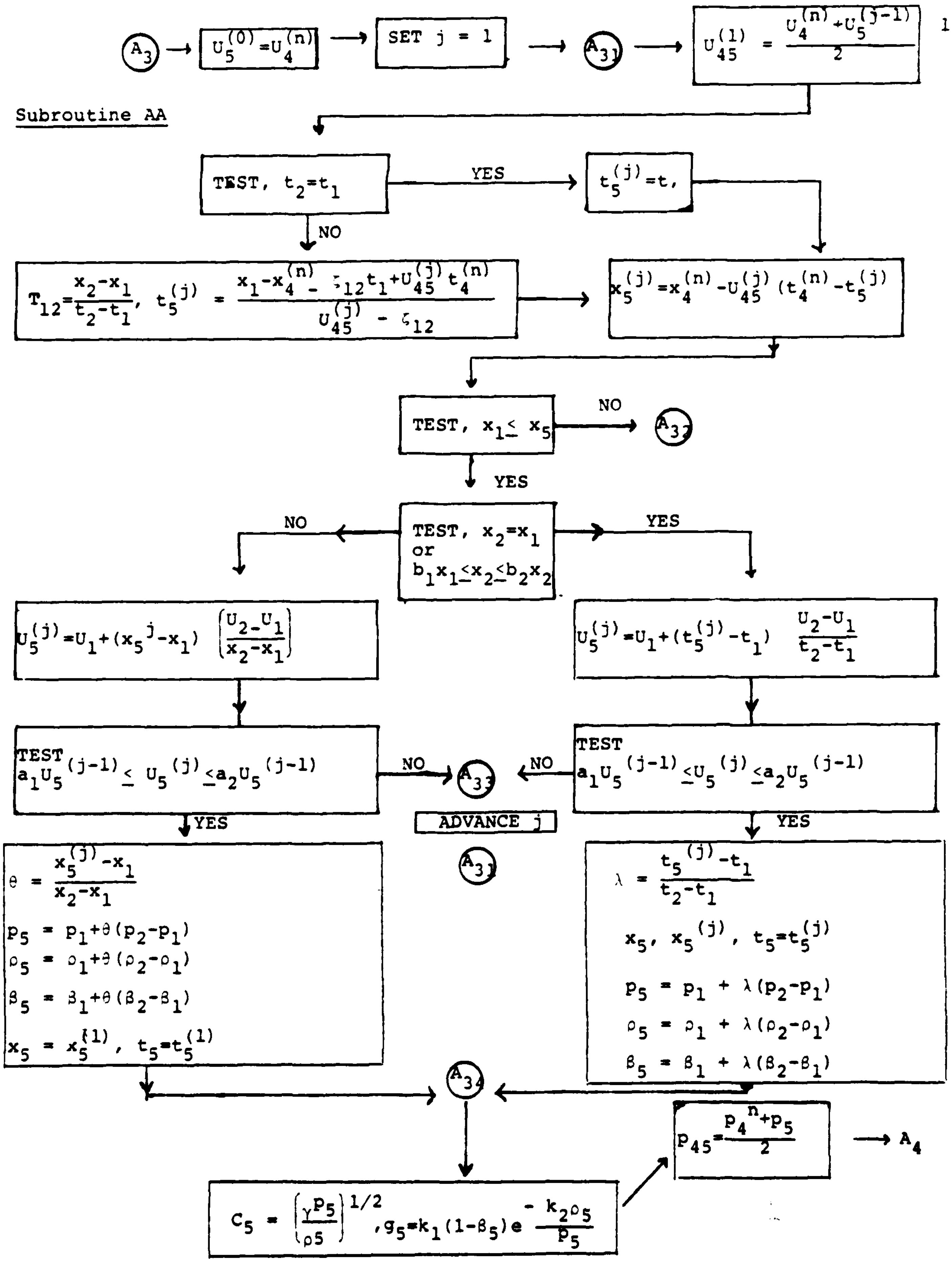
$$t_4^{(n)}=\frac{x_2-x_3+(U_{34}^{(n-1)}+C_{34}^{(n-1)})t_3-(U_{24}^{(n-1)}-C_{24}^{(n-1)})t_2}{U_{34}^{(n-1)}+C_{34}^{(n-1)}-U_{24}^{(n-1)}+C_{24}^{(n-1)}}$$

$$x_4^{(n)}=x_3+(U_{34}^{(n-1)}+C_{34}^{(n-1)})(t_4^{(n)}-t_3)$$

$$U_4^{(n)}=\frac{(\gamma-1)Q\{\rho_{34}^{(n-1)}g_{34}^{(n-1)}(t_4^{(n)}-t_3)-\rho_{24}^{(n-1)}g_{24}^{(n-1)}(t_4^{(n)}-t_2)\}+p_3-p_2+\rho_{34}^{(n-1)}C_{34}^{(n-1)}U_3+\rho_{24}^{(n-1)}C_{24}^{(n-1)}U_2}{\rho_{34}^{(n-1)}C_{34}^{(n-1)}+\rho_{24}^{n-1)}C_{24}^{(n-1)}}$$

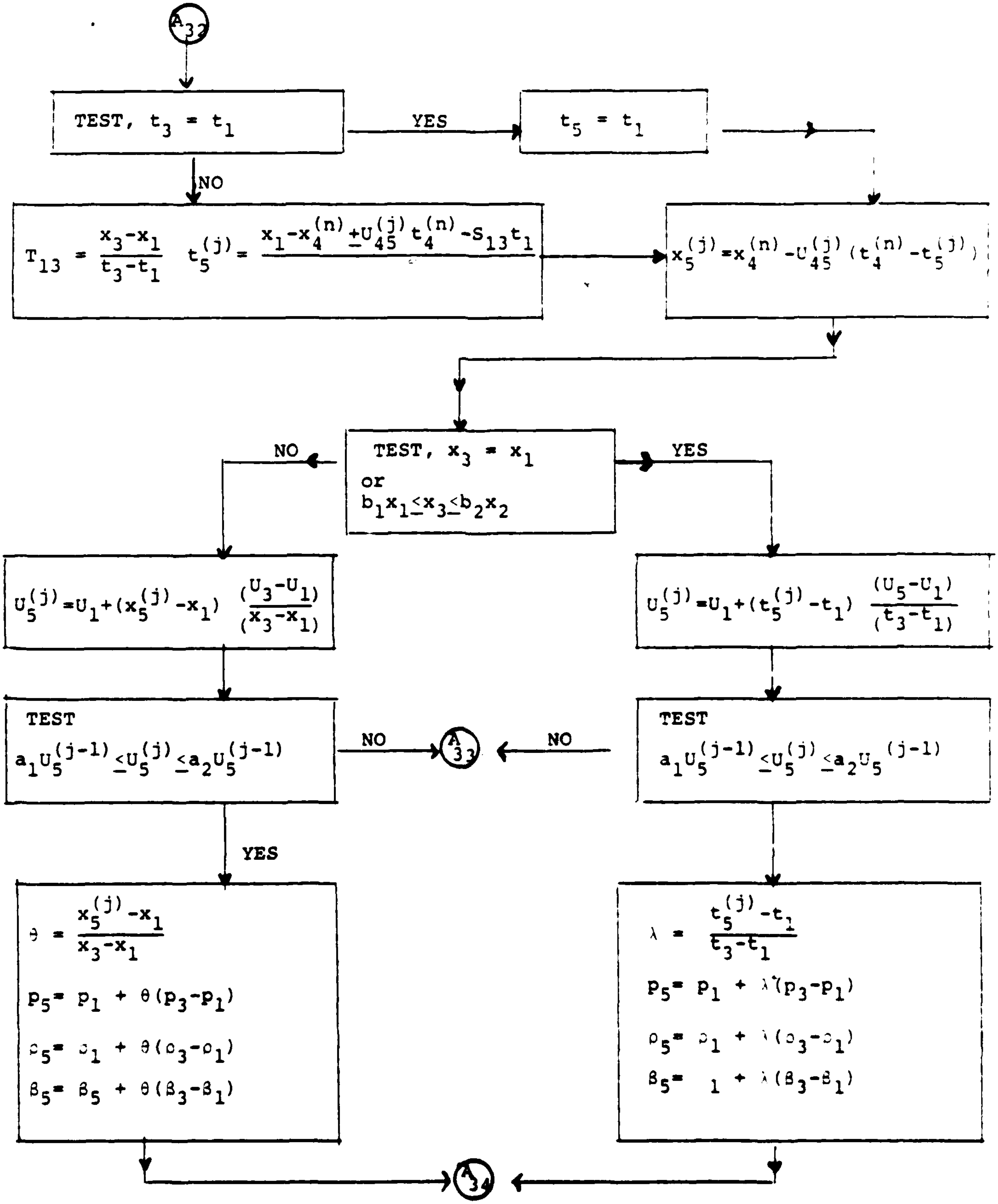
$$p_4^{(n)}=p_3-{}_{34}^{(n-1)}C_{34}^{(n-1)}(U_4^{(n)}-U_3)+(\gamma-1)Q\rho_{34}^{(n-1)}g_{34}^{(n-1)}(t_4^{(n)}-t_3)$$

$A_3$



$A_3$
$U_5^{(0)} = U_4^{(n)}$
SET j = 1
$A_{31}$
$U_{45}^{(1)} = \frac{U_4^{(n)} + U_5^{(j-1)}}{2}$
Subroutine AA
TEST, $t_2 = t_1$
YES
$t_5^{(j)} = t_1$
NO
$T_{12} = \frac{x_2 - x_1}{t_2 - t_1}$, $t_5^{(j)} = \frac{x_1 - x_4^{(n)} - \tau_{12} t_1 + U_{45}^{(j)} t_4^{(n)}}{U_{45}^{(j)} - \tau_{12}}$
$x_5^{(j)} = x_4^{(n)} - U_{45}^{(j)} (t_4^{(n)} - t_5^{(j)})$
TEST, $x_1 \le x_5$
NO
$A_{32}$
YES
TEST, $x_2 = x_1$ or $b_1 x_1 \le x_2 \le b_2 x_2$
NO
YES
$U_5^{(j)} = U_1 + (x_5^{j} - x_1) \left(\frac{U_2 - U_1}{x_2 - x_1}\right)$
$U_5^{(j)} = U_1 + (t_5^{(j)} - t_1) \frac{U_2 - U_1}{t_2 - t_1}$
TEST $a_1 U_5^{(j-1)} \le U_5^{(j)} \le a_2 U_5^{(j-1)}$
NO
$A_{33}$
NO
TEST $a_1 U_5^{(j-1)} \le U_5^{(j)} \le a_2 U_5^{(j-1)}$
YES
ADVANCE j
$A_{31}$
YES
$\theta = \frac{x_5^{(j)} - x_1}{x_2 - x_1}$
$p_5 = p_1 + \theta(p_2 - p_1)$
$\rho_5 = \rho_1 + \theta(\rho_2 - \rho_1)$
$\beta_5 = \beta_1 + \theta(\beta_2 - \beta_1)$
$x_5 = x_5^{(1)}$, $t_5 = t_5^{(1)}$
$\lambda = \frac{t_5^{(j)} - t_1}{t_2 - t_1}$
$x_5, x_5^{(j)}, t_5 = t_5^{(j)}$
$p_5 = p_1 + \lambda(p_2 - p_1)$
$\rho_5 = \rho_1 + \lambda(\rho_2 - \rho_1)$
$\beta_5 = \beta_1 + \lambda(\beta_2 - \beta_1)$
$A_{34}$
$p_{45} = \frac{p_4^{n} + p_5}{2}$
$A_4$
$C_5 = \left(\frac{\gamma p_5}{\rho 5}\right)^{1/2}, g_5 = k_1 (1 - \beta_5) e^{-\frac{k_2 \rho_5}{p_5}}$

Subroutine AA (Cont'd)



$A_4$ → Calc $\rho_4^{(n)}, g_4^{(n)}, \beta_4^{(n)}, C_4^{(n)}$

$${}_4^{(0)} = {}_5,\quad g_4^{(0)} = g_5,\quad {}_4^{(0)} = {}_5,\quad C_4^{(0)} = \left(\frac{\gamma p_4^{(n)}}{\rho_4^{(0)}}\right)^{1/2}$$

SET m = 1

$A_{41}$

$$\rho_{45}^{(m)} = \frac{\rho_4^{(m-1)} + \rho_5}{2}, \qquad C_{45}^{(m)} = \left(\frac{\gamma P_{45}}{\rho_{45}^{(m)}}\right)^{1/2}$$

$$\rho_4^{(m)} = \rho_5 + \frac{P_4^{(n)} - P_5 - (\;\; -1)Q\;{}_{45}^{(m)}\; g_{45}^{(m)}\; (t_4^{(n)} - t_5)}{[C_{45}^{(m)}]^2}$$

$$\beta_4^{(m)} = \beta_5 + g_{45}^{(m)}\;(t_4^{(n)} - t_5)$$

$$g_4^{(m)} = k_1\;(1-\beta_4^{(m)})^{\sigma}\; e^{\frac{-k_2\rho_4^{(m)}}{P_4^{(n)}}}$$

TEST, $a_1\alpha_4^{(m-1)} \le \alpha_4^{(m)} \le a_2\alpha_4^{(m-1)}$

$\alpha = \rho, \beta, g$

NO → ADVANCE m → $A_{41}$

YES

$$\rho_4^{(n)} = \rho_4^{(m)},\; g_4^{(n)} = g_4^{(m)},\; \beta_4^{(n)} = \beta_4^{(m)},\; C_4^{(n)} = \left(\frac{\gamma P_4^{(n)}}{\rho_4^{(n)}}\right)^{1/2}$$

→ $A_5$

$A_7$

$$\alpha_{34}^{(n)} = \frac{\alpha_3 + \alpha_4^{(n)}}{2}, \quad \alpha = U, \; , c$$

$$\alpha_{24}^{(n)} = \frac{\alpha_2 + \alpha_4^{(n)}}{2}, \quad \alpha = u, \rho, c$$

B

PISTON PATH POINT

$$\rho_{32}^{(0)} = \rho_2 \quad \rho_{31}^{(0)} = \rho_1 \quad x_3^{(0)} = 0 \quad \rho_3^{(0)} = 0$$

$$g_{32}^{(0)} = g_2 \quad g_{31}^{(0)} = g_1 \quad t_3^{(0)} = 0 \quad g_3^{(0)} = 0$$

$$c_{32}^{(0)} = c_2 \quad c_{31}^{(0)} = c_1 \quad p_3^{(0)} = 0 \quad \beta_3^{(0)} = 0$$

$$U_3 = U_A$$

$$U_{32} = \frac{U_A + U_2}{2}$$

SET $\ell = 1$

$B_1$

$$t_3^{(\ell)} = \frac{x_2 - x_1 + U_A t_1 - (U_{32} - C_{32}{}^{(\ell-1)})\ t_2}{U_A - U_{32} + C_{32}^{(\ell-1)}}$$

$$x_3^{(\ell)} = x_1 + U_A t_3 - U_A t_1 + U_a(t_3 - t_1)$$

F- $$p_3^{(\ell)} = p_2 + \rho_{32}^{(\ell)} \cdot C_{32}^{(\ell-1)}\ (U_A - U_2) + (\gamma-1) Q \rho_{32}{}^{(\ell-1)} g_{32}{}^{(\ell-1)} (t_3^{(\ell)} - t_2)$$

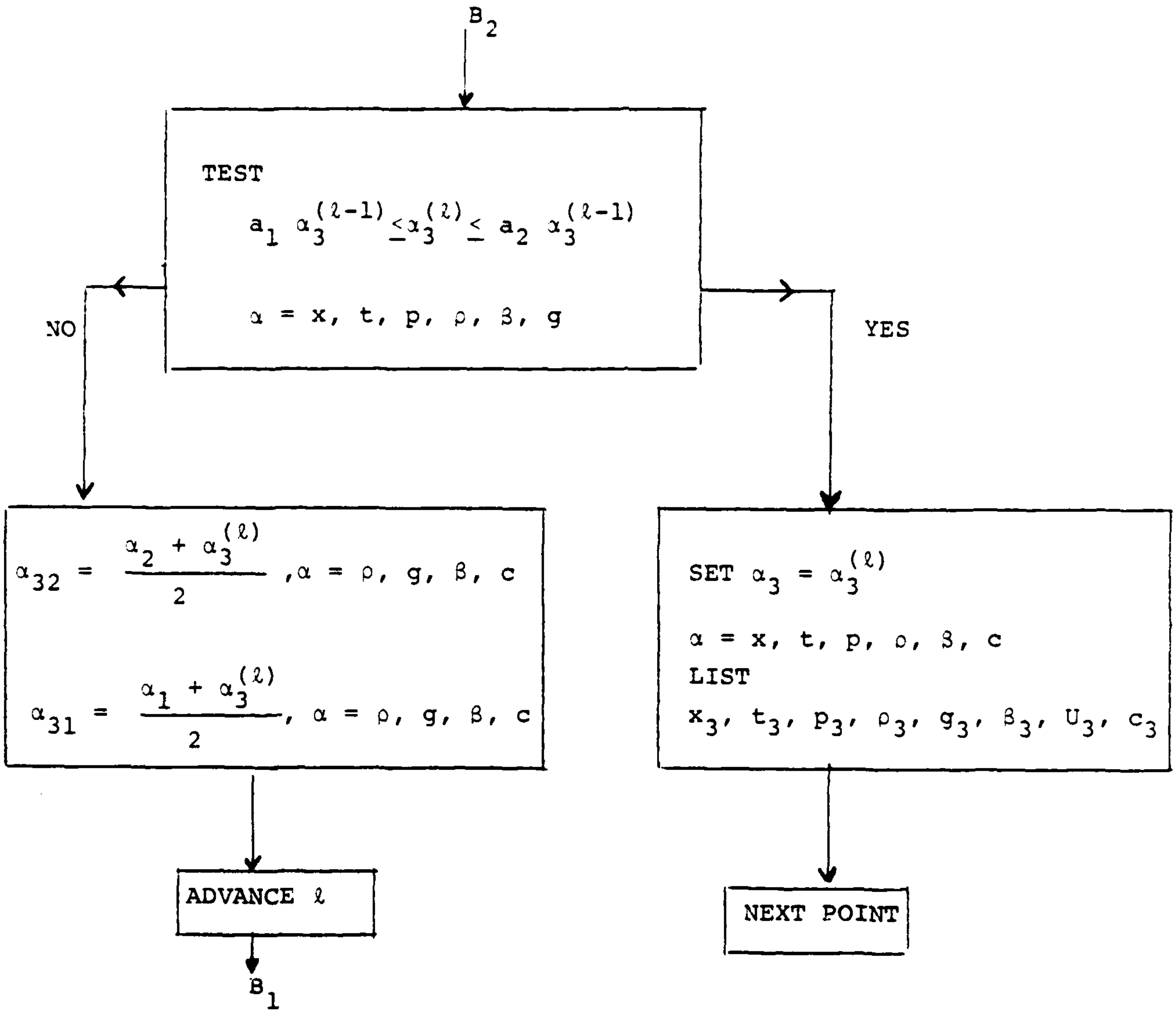
G- $$\rho_3^{(\ell)} = \rho_1 + \frac{p_3^{(\ell)} - p_1 - (\gamma-1)\ Q\ \rho_{31}^{(\ell-1)}\ (g_{31}^{(\ell-1)}\ (t_3^{(\ell)} - t_1))}{[C_{31}^{(\ell-1)}]^2 \qquad (\beta_3 - \beta_1)}$$

$$\beta_3^{(\ell)} = \beta_1 + g_{31}^{(\ell-1)}\ (t_3^{(\ell)} - t_1)$$

$$g_3^{(\ell)} = k_1\ (1 - \beta_3^{(\ell)})^{J=1} e^{\frac{-k_2\ \rho_3^{(\ell)}}{p_3^{(\ell)}}}$$

$$C_3^{(\ell)} = \left(\frac{\gamma \rho_3^{(\ell)}}{p_3^{(\ell)}}\right)^{1/2}$$

$B_2$


$B_2$
TEST
$a_1\ \alpha_3^{(\ell-1)} \le \alpha_3^{(\ell)} \le a_2\ \alpha_3^{(\ell-1)}$
$\alpha = x, t, p, \rho, \beta, g$
NO
YES
$\alpha_{32} = \frac{\alpha_2 + \alpha_3^{(\ell)}}{2}, \alpha = \rho, g, \beta, c$
$\alpha_{31} = \frac{\alpha_1 + \alpha_3^{(\ell)}}{2}, \alpha = \rho, g, \beta, c$
SET $\alpha_3 = \alpha_3^{(\ell)}$
$\alpha = x, t, p, \rho, \beta, c$
LIST
$x_3, t_3, p_3, \rho_3, g_3, \beta_3, U_3, c_3$
ADVANCE $\ell$
NEXT POINT
$B_1$

C

SHOCK POINT

**INITIALIZATION**

$U_{31}^{(0)} = U_1 \qquad \rho_3 = \frac{\gamma+1}{\gamma-1}\rho_0 \qquad U_{32}^{(0)} = \frac{U_3^{(0)}+U_2}{2}, \ \beta_3 = 0$

$C_{32}^{(0)} = C_2 \qquad \rho_{32} = \frac{\rho_3+\rho_2}{2} \qquad x_3^{(0)} = 0, \ t_3^{(0)} = 0, \ g_3^{(0)} = 0$

$g_{32}^{(0)} = g_2 \qquad U_3^{(0)} = \frac{2U_1}{\gamma+1} \qquad \rho_3^{(0)} = 0, \ U_3^{(0)} = 0, \ U_3^{(0)} = U_1$

SET $q = 1$

$C_1$

$$t_3^{(q)} = \frac{x_1 - x_2 + (U_{32}^{(q-1)} + C_{32}^{(q-1)})\, t_2 - U_{31}^{(q-1)}\, t_1}{U_{32}^{(q-1)} + C_{32}^{(q-1)} - U_{31}^{(q-1)}}$$

$$x_3^{(q)} = x_1 + U_{31}^{(q-1)}\,(t_3^{(q)} - t)$$

$$p_3^{(q)} = p_2 - \rho_{32}\, C_{32}^{(q-1)}\,(U_3^{(q-1)} - U_2) + (\gamma-1)Q\rho_{32}\, g_{32}^{(q-1)}\,(t_3^{(q)} - t_2)$$

$$g_3^{(q)} = k_1\, e^{\frac{-k_2\rho_3}{p_3^{(q)}}}, \quad C_3^{(q)} \left(\frac{\gamma p_3^{(q)}}{\rho_3}\right)^{1/2}, \quad U_3^{(q)} = \left[\frac{(\gamma+1)\,p_3^{(q)}}{2\rho_0}\right]^{1/2}, \quad U_3^{(q)} = \frac{2U_3^{(q)}}{\gamma+1}$$

TEST, $a_1\,\alpha_3^{(q-1)} \le \alpha_3^{(q)} \le a_2\alpha_3^{(q-1)}$, $\alpha = x, t, \rho, g$

NO:

$\alpha_{32}^{(q)} = \frac{\alpha_3^{(q)} + \alpha_2}{2}$, $\alpha = \rho, c, u, g, U$

ADVANCE q

$C_1$

YES:

SET $\alpha_3 = \alpha_3^{(q)}$

$\alpha = x, t, p, g, u, U$

LIST

$x_{31} t_{31} \rho_{31} g_{31} u_{31} U_{31} \beta_{31} c_{31}$ 31

NEXT POINT

3. <u>The Characteristic Equations in the Steady State</u>.

The description of the one-dimensional, steady-state, detonation of an ideal gas may be found in [4]. In this section we shall use their solution in order to obtain the steady state characteristics, $I_{+,-}$. These characteristics will be useful to us in solving for the transcient characteristics

In the undetonated region the specific enthalpy may be represented in the form [3]

$$i_0 = \frac{\gamma}{\gamma-1} p_o U_0 + Q = c_p T_0 + Q; \qquad (3.1)$$

right after the shock front (but before any reaction occurs) we represent it as

$$i = \frac{\gamma}{\gamma-1} p_1 U_1 + Q = c_p T_1 + Q. \qquad (3.2)$$

By combining these two equations we may obtain the shock condition

$$i = c_p T = \frac{(U_1+U_0)(p_1-p_0)}{2}. \qquad (3.3)$$

In the steady state situation, the reaction zone will be seen to move (with a constant velocity D) in a manner such that there is no time variation of thermodynamic variables in this region. From the equations of conservation for mass and momentum, the detonation velocity may be expressed as $D = U_0\sqrt{\frac{p_1-p_0}{U_0-U_1}}.$ (3.4)

In the case of steady state this formula, however, is valid not only for the pair $(p_1, U_1)$ <u>right after</u> the shock, but for <u>any</u> pair (p,U) in the reaction zone. From this one obtains a p,U relation for positions in the reaction zone (the Rayleight-Michelson line) [3],

$$p = p_0 + \frac{D}{U_0^2}(U_0 - U). \qquad (3.5)$$

As has been pointed out by numerous authors; see to name a few [1]-[4] the three conservation equations (mass, momentum, energy), plus the equation of state are not sufficient to uniquely determine the detonation velocity. Howver, by using the Chapman-Jouguet hypothesis the detonation velocity is given by

$$D = u + a \text{ at } \beta = 0. \qquad (3.6)$$

At a position in the reaction zone, where the fraction of nonreacting molecules is $\beta$ the enthalpy may be expressed as,

$$i = \frac{\gamma}{\gamma - 1} pU + \beta Q; \qquad (3.7)$$

if we combine this with the expression for the initial enthalpy (before detonation) one has

$$\frac{\gamma}{\gamma - 1} pU + (\beta - 1)Q = \frac{1}{2} p(U_0 + U). \qquad (3.8)$$

Combining these with the p,U relation on the Rayleigh line (and assuming $p_0$ is negligibly small) we obtain p,U in terms of the progress $\beta$, [4]

$$p(\beta) = \frac{D^2}{U_0(\gamma+1)}\left[1 \pm \sqrt{1 - \frac{2(\gamma^2-1)Q(1-\beta)}{D^2}}\right], \qquad (3.9)$$

$$U(\beta) = \frac{U_0\gamma}{\gamma+1}\left[1 \mp \frac{1}{\gamma}\sqrt{1 - \frac{2(\gamma^2-1)Q(1-\beta)}{D^2}}\right].$$

It is convenient to introduce local coordinates in the moving reaction zone, defined by a point transformation from the (x,t)-plane to the $(\xi,\tau)$-plane:

$$\xi = tD - x, \qquad (3.10)$$
$$\tau = t - \frac{x}{D}.$$

The variable $\xi$ is the distance from a position x to the shock front, whereas $\tau$ is the time that has elapsed after the front has passed the point x. We may express $\xi$ and $\tau$ in terms of $\beta$ by means of a single quadrature as follows. From equation we have

$$\dot\beta \equiv g(\rho,p,\beta) = g\left(\frac{1}{U(\beta)}, p(\beta), \beta\right) \equiv \phi(\beta), \qquad (3.11)$$

consequently upon integration one has

$$\tau = \int_0^\tau d\tau = \int_1^\beta \frac{d\beta}{\phi(\beta)} = \mathcal{F}(\beta), \qquad (3.12)$$

and

$$\xi = \int_0^{\xi} d\xi = \int_1^{\beta} \frac{[D-u(\beta)]}{\phi(\beta)} d\beta \equiv \mathfrak{J}(\beta) \qquad (3.13)$$

where

$$u(\beta) = [p(\beta)-p_0][U_0- (\beta)] \cong p(\beta) [ _0- (\beta) ]. \qquad (3.14)$$

Elimating $\beta$ between $\tau = \mathfrak{T}(\beta)$ and $\xi = \mathfrak{J}(\beta)$, yields an expression for $\xi$ in terms of $\tau$, $\xi = \mathfrak{J}[\mathfrak{T}^{-1}(\tau)]$.

In the steady-state it is clear that the characteristic lines, $I_+$, correspond to the straight lines $\beta$= constant, or $I_+ : x = tD + (\beta-1)L$, where L is the reaction zone length. In order to obtain $I_-$, we return to equation (1.8) $I_-: \frac{dx}{dt} = u(\beta) - a(\beta)$, and compute $a(\beta)$ from

$$a^2(\beta) = \left(\frac{\partial p}{\partial p}\right)_s \doteq \gamma p(\beta) v(\beta), \qquad (3.15)$$

$$a(\beta) = \frac{D\gamma}{\gamma-1}\sqrt{\frac{2(\gamma^2-1)(1-\beta)Q}{D} + \left(1-\frac{1}{\gamma}\right)\left(1 \pm\sqrt{1 - \frac{2(\gamma^2-1)(1-\beta)Q}{D^2}}\right)} \qquad (3.16)$$

Consequently, on $I_-$, the slope $\frac{dx}{dt}$ is given as the following function of $\beta$

$$\frac{dx}{dt} = \frac{D^2\gamma^2}{(\gamma-1)^2}\left[\frac{2(\gamma^2-1)(1-\beta)Q}{D^2} + \left(1-\frac{1}{\gamma}\right)\left(1 \pm\sqrt{1 - \frac{2(\gamma^2-1)(1-\beta)Q}{D^2}}\right)\right]$$

$$- \frac{D\gamma}{\gamma-1}\sqrt{\frac{2(\gamma^2-1)(1-\beta)Q}{\gamma^D} + \left(1-\frac{1}{\gamma}\right)\quad 1 \pm\sqrt{1 - \frac{2(\gamma^2-1)(1-\beta)Q}{D^2}}} \qquad (3.17)$$

It is clear from the above discussion that all the "cross-characteristics," $I_-$, cut the lines $\beta$=constant at the same angle, and hence the $I_-$ form a "parallel" family of curves. From the information connecting $\xi$, $\tau$, and $\beta$ we may start at the shock front, compute the slope of $I_-$, and then proceed by finite differences across the reaction zone. The computation of one cross-characteristic will then yield the entire family.

4. A Progressing Wave Interpretation:

In this section we attempt to solve the system of partial differential equations (1) (2) (3) (4) in terms of a similarity variable [1] [4] $\xi = xt^{-\alpha}$. We introduce this variable in order to reduce a system of partial differential equations to a system of ordinary differential equations.* We make the assumption that the solutions u, $\rho$, p, have the form

$$
\begin{aligned}
u &= \alpha x t^{-1} U(\xi), \\
\rho &= x^k \Omega(\xi),
\end{aligned}
\tag{4.1}
$$

and

$$p = \alpha^2 x^{k+2} t^{-2} P(\xi).$$

In addition we introduce,

$$\beta = B(\xi),$$

and

$$e = \frac{\alpha^2 x^2 t^{-2}}{\gamma - 1} \frac{P(\xi)}{\Omega(\xi)} = \frac{\alpha^2 x^2 t^{-2}}{\gamma - 1} E(\xi). \tag{4.2}$$

*We note, however, that these solutions cannot approach the steady-state case discussed earlier, since here the reaction zone continues to grow in length.

Equations 1.1, 1.2 may then be written respectively as

$$(U-1)\xi\Omega' + KU\Omega + \Omega[U+\xi U'] = 0, \qquad \text{(4.3)}$$

$$U(\alpha U-1) + \alpha\xi U'(U-1) + \alpha(k+2)\frac{P}{\Omega} + \frac{\alpha\xi P'}{\Omega} = 0, \qquad \text{(4.4)}$$

where primes indicate differentiation with respect to $\xi$. Equation 1.3 becomes

$$Q\xi B' = \alpha x^2 t^{-2}\,\frac{2(\alpha-1)}{\gamma-1}\,E - \frac{\alpha P}{\Omega^2}\quad(U-1)\xi\Omega' + KU\Omega) \quad , \qquad \text{(4.5}$$

and then in order for B to be a function of $\xi$ alone we must have $\alpha = 1$, or $\xi = \frac{x}{t}$. Equation 1.4 reduces to

$$\alpha\xi(U-1)B' = tg(\rho,p,\beta); \qquad \text{(4.6)}$$

consequently, for there to exist a similarity solution (progressing wave) for our case $tg(\rho,p,\beta)$ must be expressible solely as a function of $\xi$. This amounts to a mathematical restriction on the type of rate function we may use; however, as we shall see, it does not impose an important physical restriction. For instance, it is customary to use rate functions of the form [3] [4]

$$\dot{\beta} = c\beta^m\rho^\ell \exp\left[-\frac{\varepsilon_0}{\varepsilon}\right] \qquad \text{(4.7)}$$

where $\varepsilon_0$ is an activation energy. In this case equation (3.6) becomes

$$\alpha\xi(U-1)B' = tc\beta^m\, x^{k\ell}\Omega^\ell \exp\frac{(1-\gamma)\quad 0}{\xi^2 E(\xi)}\,, \qquad \text{(4.8)}$$

which will be an expression in $\xi$ alone, if $x^{k\ell}t = \xi^{-1}$ or $k = -\frac{1}{\ell}$, $\ell \neq 0$. The system (4.1) - (4.4) then takes on the form

$$(U-1)\xi\Omega' - \frac{1}{\ell}\Omega + \Omega[U+\xi U'] = 0,$$

$$\Omega(U-1)\ [U+\xi U'] + \xi P' + (2-\frac{1}{\ell})P = 0,$$

$$Q\xi\Omega^2 B' + \xi^2 P[(U-1)\xi\Omega' - \frac{1}{\ell}U\Omega] = 0,$$

and

$$\xi^2(U-1)B' = cB^m\Omega^\ell \exp\frac{(1-\gamma)\varepsilon_0}{\xi^2 E(\xi)}. \qquad (4.9)$$

This system may be solved for the first derivatives $U'$, $\Omega'$, $P'$, $B'$, as follows

$$U' = \frac{1}{\xi(U-1)}\left\{-U+cQ\Omega^{\ell+1}B^m \exp\left[\frac{(1-\gamma)\varepsilon_0\Omega}{\xi^2 P}\right]\right\}, \qquad (4.10)$$

$$\Omega' = \frac{U\Omega}{\ell\xi(U-1)} - \frac{cQ\Omega^{\ell+2}B^m}{\xi^4(U-1)^2 P}\exp\left[\frac{(1-\gamma)\varepsilon_0\Omega}{\xi^2 P}\right], \qquad (4.11)$$

$$P' = (\frac{1}{\ell}-2)\frac{P}{\xi} - cQ\Omega^{\ell+2}B^m \exp\left[\frac{(1-\gamma)\varepsilon_0\Omega}{\xi^2 P}\right], \qquad (4.12)$$

$$B' = \frac{cB^m\Omega^\ell}{\xi^2(U-1)}\exp\left[\frac{(1-\gamma)\varepsilon_0\Omega}{\xi^2}\right]. \qquad (4.13)$$

The equations (4.10), (4.11), (4.12), (4.13) are a system of four ordinary differential equations in four dependent variables. The four equations are essentially different as is illustrated by solving for $U'$, $\Omega'$, $P'$, $B'$, and may be solved by numerical methods.

## References


1. Courant, R. and Friedrichs, K. O.: Supersonic Flow and Shock Waves, Springer Verlag, Heidelberg, 1948.

2. Jeffrey, A.: Quasilinear Hyperbolic Systems and Waves, Pitman Publishing, London, 1976.

3. Soloukhin, R. I.: Shock Waves and Detonation in Gases, trans. B. W. Kuvshinoff, Mono Book Co., Baltimore, 1966.

4. Zel'dovich, Ya. B. and Raizer, Yu P.: Elements of Gasdynamics and the Classical Theory of Shock Waves, Academic Press, New York, 1966.

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