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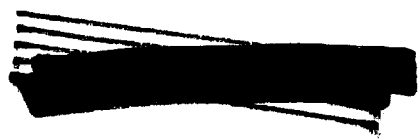


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NUMERICAL METHODS

Volume Editor: E. Nelson

Part II

Chapters 6 through 8

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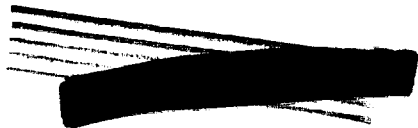
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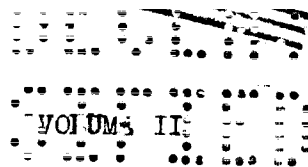
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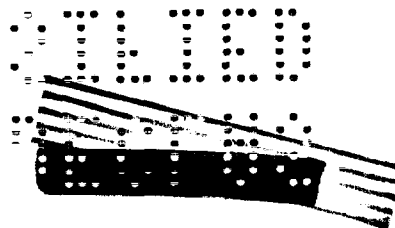
NUMERICAL METHODS

Volume Editor: E. Nelson

Part II

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NUMERICAL INTEGRATION OF PARTIAL DIFFERENTIAL EQUATIONS

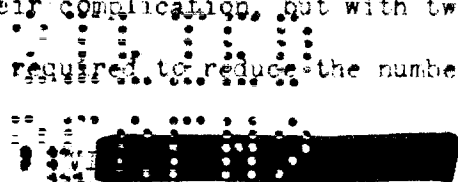
Nelson, R. Peierls, T. H. R. Skyrme

6.1 INTRODUCTION AND EQUATIONS (T.H.R. Skyrme)

In the numerical integration of ordinary differential equations, as discussed in the last chapter, we have to find the value of one or more functions $f(x)$ in a sequence of n values of the independent variable x ; for problems of similar type the labour required is proportioned to n . In the integration of a partial differential equation, we require the values of a function $f(x_1, x_2, \dots)$ at a set of n_r values of each of the m independent variables x_r . Usually the process of integration will require that all the n_r be of the same order of magnitude, n , even though we may not wish to know the value of $f(x_r)$ for all these values, and consequently the labour required is proportioned to n^m .

Now in any problem in which the values of the dependent variables vary significantly over the range of integration (and all interesting problems are of this type) accurate results may be obtained only if n be a large number. The first consequence of this is that the effort needed increases enormously with the number m of independent variables; even with the assistance of I.B.M. machines tolerably accurate solution to problems with $m > 2$ cannot, in practice, be obtained within a reasonably short time. The subsequent discussion is, therefore, limited to the case $m=2$, with two independent variables.

Secondly, the large number of operations required limits severely the completion of each operation. As in the integration of ordinary differential equations, there is some choice between decreasing the number of operations and decreasing their complication, but with two independent variables the complications required to reduce the number of operations



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while retaining the same accuracy generally outweigh the gain, especially when the calculations are carried out by machines. If, however, we can sacrifice some accuracy there may be an overall gain.

This brings us to the third point, namely, that in two-variable problems there is a much greater premium on accuracy. In fact, it is very difficult to estimate the absolute accuracy obtainable with a given method of integration, and the necessary magnitude of n has been found mainly by experimentation with particular problems.

§.1-1 Hydrodynamical Equations.

This chapter is concerned mainly with the integration of one particular partial differential equation, that of the radially symmetric flow of a fluid in space. Analogous methods would, however, exist for many partial differential equations of the second order of "hyperbolic" type; that is, equations having real characteristics and which can therefore be solved by a step-by-step integration process.

The equations of symmetrical motion of a fluid in space of k dimensions ($k = 1, 2, 3$) may be formulated in two ways, from which the two principal methods of integration are desired. In the first, or Lagrangean system, the independent variables are the time t , and a label coordinate ξ for the particle; the dependent variable is the distance R from a fixed origin of the particle ξ at any time t . It is convenient to choose for ξ either the original position, r , of the particle before the fluid began to move

$$r = R(\xi, 0) \quad (1)$$

or a "mass variable" m defined by

$$m = \int \rho_0 d[R^k(\xi, 0)] \quad (2)$$

where ρ_0 is the original density of the fluid in the neighborhood of the

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particle ξ . (The actual mass differs by a factor π or $\frac{4\pi}{3}$, for $k = 2, 3$).
 With this notation the equation of motion of the fluid is

$$\frac{\partial^2 R}{\partial t^2} = - \left(\frac{R}{r} \right)^{k-1} \rho_0 \frac{\partial p}{\partial r} = - (kR^{k-1}) \frac{\partial p}{\partial m} \quad (3)$$

where p is the pressure at the point r, t . The pressure is some given function of the specific volume v (equal to the reciprocal of the density) and the entropy S . So long as the motion is continuous and heat condition is neglected $\frac{\partial S}{\partial t} = 0$ and S will be a function only of the label r or m , determined by the boundary conditions (a particle will only enter the field of integration after it has crossed some boundary). The specific volume v is given by the equation

$$v = \frac{1}{\rho_0} \left(\frac{R}{r} \right)^{k-1} \frac{\partial R}{\partial r} = \frac{\partial R^k}{\partial m} \quad (4)$$

The second, or Eulerian, formulation of the hydrodynamical equations regards as independent variables t and R , and as dependent variables the velocity u , pressure p , density ρ . The equation of motion then takes the form

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial R} + \frac{1}{\rho} \frac{\partial p}{\partial R} = 0 \quad (5)$$

while Equation (4) is replaced by its time derivative, the equation of continuity

$$\frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial R} + \rho \left(\frac{\partial u}{\partial R} + \frac{(k-1)u}{R} \right) = 0 \quad (6)$$

6.1-2 Characteristics.

The local "sound velocity" at any point in the fluid is

$$c = \sqrt{(\partial p / \partial \rho)_S} \quad (7)$$

If an infinitesimally weak disturbance be superimposed on the main motion of the fluid, this disturbance will spread in all directions from any point with the local sound velocity relative to the fluid. A disturbance

localized at a point R_0 at one time t_0 ; then, after an interval of time Δt , be confined within the interval $R_0 - (u+c)\Delta t \leq R \leq R_0 + (u+c)\Delta t$ where u, c have their values at R_0, t_0 . It is clear, therefore, that this small disturbance must always remain within the limits defined by the two paths in (R, t) space, passing through (R_0, t_0) , that are the solutions of the two differential equations

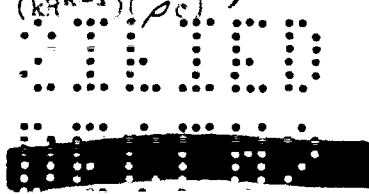
$$\frac{dR}{dt} = u \pm c \tag{8}$$

The two one-parameter families of curves defined by these equations in (R, t) space are called the characteristics. It can be shown that they limit the region over which any disturbance (not necessarily small) can spread, provided only that no discontinuities are formed in the fluid. If the fluid motion be known up to a certain time t_0 over the interval $R_1 \leq R \leq R_2$, then, provided there are no discontinuities, the differential equations will define the subsequent motion only over a region that is the least region bounded by characteristics passing through R_1, R_2 for which $t > t_0$; and, conversely, the motion at any point in this region is determined by conditions within an appropriate subinterval of (R_1, R_2) .

This property of the characteristics is most important for the numerical integration. For, clearly, no method of integration can give correct results that attempts to calculate, from the interval $(R_1 \leq R \leq R_2)$ at time t_0 , the values of the variables without the region bounded by characteristics through R_1, R_2 ; in fact, the attempt to do so will lead to instability as is shown below in 6.4.

In terms of the Lagrangean variables of Section 6.1-1, the paths of the characteristics in (r, t) or (m, t) space are given by

$$\left. \begin{aligned} \frac{dr}{dt} &= \left(\frac{R}{r}\right)^{k-1} \left(\frac{\rho_0}{\rho}\right) \\ \frac{dm}{dt} &= (kR^{k-1}) \left(\frac{\rho_0}{\rho}\right) \end{aligned} \right\} \tag{9}$$



The only discontinuity that can arise in the types of motion considered here is a shock wave, that is to say, a surface in the fluid across which the pressure and material velocity change discontinuously. Such a discontinuity moves relative to the fluid with a velocity which is greater than the local sound velocity ahead of the shock and less than that behind (otherwise the discontinuity would be unstable and break up into ordinary sound waves). Since it is supersonic with respect to the fluid ahead it will advance more rapidly than the characteristics which go in the same direction and which therefore are gradually eaten up. Consequently the motion of the fluid ahead of the shock (but not the limit of continuous motion) is determined independently of the presence of the shock. When conditions ahead of the shock are known, there is one free parameter in the values of the hydrodynamical variables behind the shock in terms of which all quantities may be expanded by use of the Rankine-Hugoniot equations⁽¹⁾. This one extra condition needed to define the motion of the shock is provided by the characteristics that reach the shock from behind. (The shock is subsonic with respect to the fluid behind it.) The characteristics of the opposite system suffer a discontinuous change in direction on crossing the shock. The situation is illustrated in Figure 1.

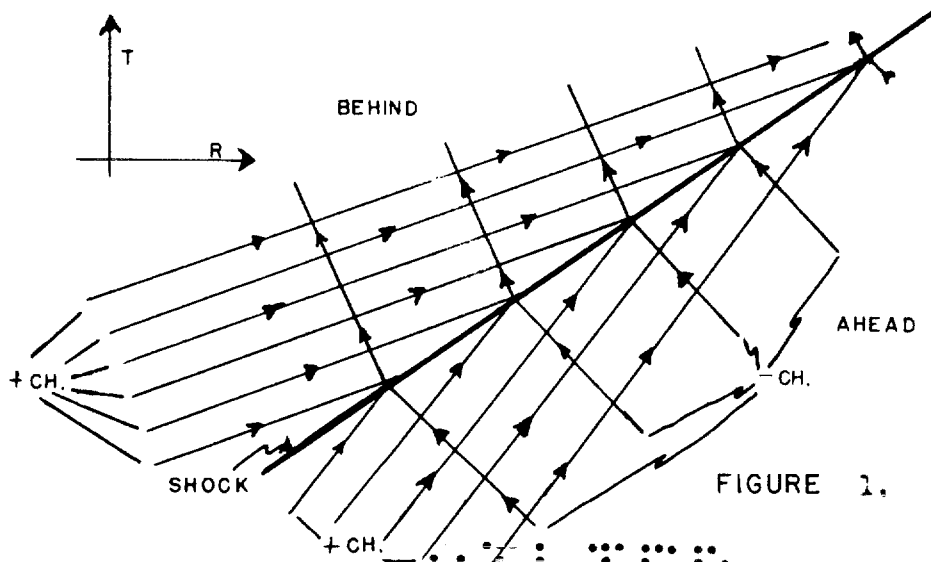


FIGURE 1.

(1) See Section 6.2-1 below.

6.1-3 One Dimension: Riemann Method.

The method of integration based on the Eulerian equations (5) and (6) is essentially a generalization of the well-known method of integration of the equations when $k = 1$, (line), and when the pressure is a unique function of the density (or the entropy is constant), developed by Riemann. It will be useful to outline the theory here for later reference.

If we multiply Equation (6), with $k = 1$, by c/ρ and add to Equation (5) we find

$$\frac{\partial u}{\partial t} + (u + c) \frac{\partial u}{\partial R} + \frac{c}{\rho} \frac{\partial \rho}{\partial t} + \frac{uc}{\rho} \frac{\partial \rho}{\partial R} + \frac{1}{\rho} \frac{\partial p}{\partial R} = 0 \quad (10)$$

If p is a unique function of ρ then $\frac{\partial p}{\partial R} = c^2 \frac{\partial \rho}{\partial R}$, and if we introduce Riemann's function

$$\sigma = \int_v^{\rho} \frac{c d\rho}{\rho} = \int_v (\rho c) dv \quad (11)$$

(where the lower limit of integration is arbitrary) then we can write

Equation (10) in the form

$$\frac{\partial (u + \sigma)}{\partial t} + (u + c) \frac{\partial (u + \sigma)}{\partial R} = 0 \quad (12)$$

Similarly,

$$\frac{\partial (u - \sigma)}{\partial t} + (u - c) \frac{\partial (u - \sigma)}{\partial R} = 0 \quad (13)$$

These equations state that along the characteristics with slope $(u \pm c)$, $(u \pm \sigma)$ is constant. In some special cases (when $p \propto \rho^\gamma$ and γ has certain values) these equations can be solved analytically and the problem is reduced to the solution of ordinary differential equations presented by the boundary conditions; generally, however, step-by-step numerical integration is needed.

In such a numerical integration we do, in effect, regard $u \pm \sigma$ as the independent variables, from which $u \pm c$ are calculable, and R, t as the dependent variables. It is most convenient to picture the steps of integration in the (R, t) plane across which the characteristics form

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another coordinate network of values of u and σ . Thus, if we know the values of u and σ in an interval $R_1 \leq R \leq R_2$ at time t_0 , we subdivide this interval by points P_i , so that the variations of u or σ between two adjacent points are small, and construct lines having slopes $u \pm \sigma$ through all the P_i . Consecutive characteristics of opposite systems will then meet in points Q_i whose (R, t) coordinates may be found from the slopes of the intersecting characteristics and whose $(u \pm \sigma)$ coordinates are determined by the particular characteristics that intersect.

This enables us to find R, t, u, σ at all the points Q_i , which can then be taken as base points for the next step in the integration. The process is illustrated in Figure 2.

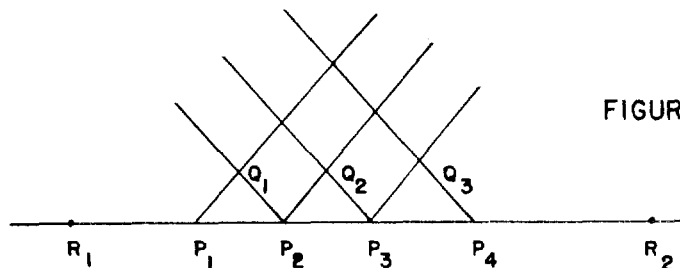


FIGURE 2.

We omit any further details here as the procedure is well known, and indeed can be regarded as a special case of the procedures discussed in Section 6.3.

6.1-4 Methods of Integration.

We shall now deal exclusively with the equations for radially symmetric motion in space, $k = 3$. It is natural to try to generalize the method of Riemann to this case. However, the additional term, $2\rho u/R$, in Equation (6) causes to appear a term $\pm 2uc/R$ on the right-hand sides of (12) and (13) so that $u \pm \sigma$ are no longer conserved along the characteristics. Indeed there is no function of the variables u and σ that is conserved along the characteristics in this case (not even in the plane case when the entropy is not constant.)

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Nevertheless, it will be convenient often to think of the characteristics as if they carried with them the value of some function, as $u \pm \sigma$, so that the physical conditions, velocity and pressure, at a point are determined by the intersection of two particular characteristics. In general, the conditions at the point are dependent not only on the particular characteristics but on the path followed by them, although their 'conservation property' is still true over infinitesimal distances. A method of integration can indeed be devised which takes these factors into account, and this is the subject of Section 6.3 below.

While this method is, in some ways, the most natural inasmuch as we follow the paths of the signals that determine the fluid motion, the operations to which it leads are somewhat complex; in practice, therefore, their number is restricted and the accuracy limited. The most useful application will usually lie in exploratory work where the qualitative features of the motion are more important than the quantitative.

When, however, I.B.M. machines are available, greater accuracy is obtainable with the same effort by a method which uses a large number of relatively simple operations; such a one is most conveniently based on the Lagrangean Equations (3) and (4) and this is described in detail in Section 6.4 below. Because, however, this integration follows paths different from the characteristics, certain of the boundary conditions are troublesome to handle. This forms a large part of the subject of the following Section 6.2.

These two methods represent somewhat extreme positions in the balance between number and simplicity of operations. It seems, however, that an intermediate type would be both too tedious for manual calculation and too complex for the present scope of mechanical computations; though with the development of the latter, the optimum may well shift in this direction.

There remains one very different way of handling the partial diff-

differential equation. When the integration of several problems of a similar type has been made, it may be found that the solutions can be represented (approximately) in some rather simple quasi-analytic form. For example, it might be that the pressure gradient was nearly constant in space, so that the pressure at any time and place could be expressed in terms of two numerically-given functions of the time. If such is the case we may try to solve another problem of the same type by assuming the same quasi-analytic form for the solution, and it may be possible to choose this in such a way that the whole problem can be reduced to the solution of a system of ordinary differential equations. These equations would be suitable averages of the true equations, chosen, if convenient, by a variational principle. When, however, this has been tried in practice, the resulting equations have been so complicated as to outweigh the advantages which might otherwise be expected from this approach.

6.2 BOUNDARY CONDITIONS (Skyrme)

The boundary conditions needed to determine the solution of our differential equation are simple in theory. If the integration starts at time t_0 over an interval $R_1 \leq R \leq R_2$, we must know the initial velocity, pressure and entropy or density distribution over this interval; then, unless discontinuities form, the solution is determined over the region bounded by characteristics through R_1, R_2 . If we desire to extend the solution beyond either of these boundaries, then we must supply one additional condition at the boundary of the field of integration to replace the information supplied by characteristics coming from without the field which must be equivalent to one relation, explicit or implicit, between the hydrodynamical variables at each instant of time.

The boundaries of such a region within which the integration is continuous may be paths along which a condition is prescribed a priori; or interfaces between two media; or discontinuities in the fluid motion, that is shock-wave fronts

Suppose first, for example, that the motion of the particle which is at R_1 at time t_0 is given. Then at every time we shall know the velocity for a certain value of the radius R . If we combine this information with that supplied by the characteristic coming from within the field of integration, we can determine ⁽¹⁾ the pressure at the point and thereby extend the field of

(1)

Speaking rather loosely in the sense mentioned - Section 6.1-4

integration to this point.

Now suppose that R_1 were the boundary point between two media and that the motion of the medium in $R \leq R_1$ is also being found by numerical integration. Now if the motion of this interface point were prescribed as in the preceding paragraph, then we could at every instant determine the pressure on either side of it by integration from that side. These pressures must be equal, however, and this imposes one condition at every instant sufficing to determine the unknown motion of the interface.

We have stated this interface problem in a somewhat elaborate way as this is the form in which it appears when we integrate along characteristics to find the field of velocity and pressure. As such it will be elaborated upon in Section 6.3. But when we are integrating in Lagrangean variables to find R as function of time and particle coordinate, an interface presents no difficulty. So long as the acceleration of the interface point is properly related to the pressure gradient across the interface, the boundary conditions look after themselves. This will be touched upon again in Section 6.4. It is clear from this that the latter method of integration is preferable when the problem involves several interfaces.

The Lagrangean method has however no such advantage when we deal with shock wave boundaries, and the rest of this section deals with this problem.

Let us suppose that at time t_0 a shock is moving in the same outward dir-

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tion as the \pm characteristics and is initially at $R=R_2$. For definiteness ⁽²⁾

(2)

If not, the motion of the fluid ahead may be determined first and the same argument then applies.

Let us suppose that the fluid ahead of the shock is at rest at constant pressure. If now the velocity of the shock, and therefore its path, were known as function of time, then the pressure and material velocity behind the shock, being functions of the shock velocity, would also be known. But through every point of the path of the shock there passes a \pm characteristic coming from within the field of integration ⁽³⁾ which determines a relation between these quanti-

(3)

See end of Section 6.1-2.

ties. This provides information to determine the values of all quantities at the shock as functions of time.

This is the principle followed when integrating along characteristics, and it is elaborated in Section 6.3. When using the Lagrangean equations we naturally do not wish to find the paths of characteristics explicitly. Instead we shall relate the motion of the shock to the gradients of pressure and density behind it. In this way we leave a small gap between the shock path and the edge of the field of integration, and this is bridged by relations derived from a combination of shock conditions with the ordinary hydrodynamic equations. This is discussed further in the following subsections together with related problems arising when the shock wave crosses an interface.

6.2-1 Conditions Across a Shock-Front.

When we are dealing with a single shock we shall use the following notation. Pressure, specific volume, sound velocity, material velocity,

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shock velocity are denoted by p, v, c, u ; U and subscripts 1, 2 refer to the low- and high-pressure sides of the shock, respectively. Then p, v, u are known functions of time and position and the Rankine-Hugoniot shock conditions determine two relations between p_2, v_2, u_2 : first the energy conservation ⁽⁴⁾

(4)

The equation is $(1/2)(p_2 + p_1)(v_1 - v_2) = E_2 - E_1$ where E denotes the internal energy, a function of p and v . If we neglect the change of entropy across the shock, $p = P(v)$ is simply the adiabatic relation.

determines

$$p_2 = P(v_2; p_1, v_1) \quad (14)$$

and the other conditions determine that

$$(u_1 - u_2)^2 = (p_2 - p_1)(v_1 - v_2) \quad (15)$$

The shock velocity is related to these by the equations

$$U = u_1 + v_1 \sqrt{\frac{p_2 - p_1}{v_1 - v_2}} = u_2 + v_2 \sqrt{\frac{p_2 - p_1}{v_1 - v_2}} \quad (16)$$

Instead of shock velocity in space it is more convenient to consider the velocity of the shock relative to the mass of the material divided by

$$4 \pi R^2, \quad W_{12} = \sqrt{(p_2 - p_1) / (v_1 - v_2)} \quad (17)$$

W_{12} has then the dimensions (density x velocity). Analogously, it will be convenient to introduce the acoustic impedances w_i , defined by

$$w_i = c_i / v_i = \left(-(\partial p / \partial v)_s \right)^{1/2} \quad (18)$$

The stability of the shock requires the condition

$$w_1 < W_{12} < w_2 \quad (19)$$

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A very useful relation is found by differentiating equation (15) with respect to time along the path of the shock. If we denote such differentiation by the symbol d/dt , and divide this equation by $(v_1 - v_2)$ after differentiation, we obtain

$$2 \left(\frac{u_1 - u_2}{v_1 - v_2} \right) \left(\frac{du_1}{dt} - \frac{du_2}{dt} \right) = \left(\frac{dp_2}{dt} - \frac{dp_1}{dt} \right) + \left(\frac{p_2 - p_1}{v_1 - v_2} \right) \left(\frac{dv_1}{dt} - \frac{dv_2}{dt} \right) \quad (20)$$

This may be rearranged and written in the form

$$X_2 = X_1 \quad (21)$$

where X_1 denotes a combination of derivatives on the i- side of the shock,

$$X_1 = W_{12}^2 \frac{dv_i}{dt} - \frac{dp_i}{dt} + 2W_{12} \frac{du_i}{dt} \quad (22)$$

When the pressure is a unique function of density

$$X_1 = (W_{12}^2 - w_i^2) \frac{dv_i}{dt} + 2W_{12} \frac{du_i}{dt}$$

The expression (22) for X_1 may be transformed in a number of ways by combination with the equations of motion and continuity. Using only the spatial derivatives of

$$X_1 = (3W_{12}^2 + w_i^2) \left(v \frac{\partial u}{\partial R} \right)_i + W_{12}^3 \left(v \frac{\partial v}{\partial R} \right)_i - 3W_{12} \left(v \frac{\partial p}{\partial R} \right)_i + \frac{2u_i v_i}{R} (W_{12}^2 - w_i^2) \quad (23)$$

An intermediate form which is useful is

$$X_1 = (3W_{12}^2 + w_i^2) \frac{dv_i}{dt} - W_{12} (2W_{12}^2 + w_i^2) \left(v \frac{\partial v}{\partial R} \right)_i - 3W_{12} \left(v \frac{\partial p}{\partial R} \right)_i - \frac{4u_i v_i}{R} W_{12}^2 \quad (24)$$

If we wish to transform so as to have time derivatives (at constant mass), rather than space derivatives, we must introduce the entropy gradient. Let S denote the entropy or some function of it, then we find

$$X_1 = - \left(1 + 3 \frac{W_{12}^2}{w_i^2} \right) \left(\frac{\partial p_i}{\partial t} \right)_m + W_{12} \left(3 + \frac{3W_{12}^2}{w_i^2} \right) \left(\frac{\partial u_i}{\partial t} \right)_m - \frac{4u_i v_i}{R} W_{12}^2 + \frac{W_{12}^3}{w_i^2} \left(\frac{\partial p}{\partial S} \right)_{v=v_i} \left(v \frac{\partial S}{\partial R} \right)_i \quad (25)$$

When we cannot neglect changes of entropy, we shall have to consider also the result of differentiating Equation (14) along the shock. We can write this as

$$\frac{dp_2}{dt} = -W_h^2 \frac{dv_2}{dt} + A \quad (26)$$

Where $A = (\partial p_2 / \partial v_1)(dv_1/dt) + (\partial p_2 / \partial p_1)(dp_1/dt)$ can be considered as known; if conditions ahead of the shock are constant, $A = 0$. Then Equation (24) may also be written as

$$X_2 = (3W_{12}^2 + W_h^2) \frac{dv_2}{dt} - 2W_{12}^3 \left(v \frac{\partial v}{\partial R}\right)_2 - 2W_{12} \left(v \frac{\partial p}{\partial R}\right)_2 - \frac{4u_2 v_2}{R} W_{12}^2 - A \quad (27)$$

We can also eliminate the entropy gradient from Equation (25)

$$X_2 = - \left(1 + \frac{2W_{12}^2}{W_2^2} + \frac{W_{12}^2}{W_h^2}\right) \left(\frac{\partial p_2}{\partial t}\right)_m + W_{12} \left(3 + \frac{W_{12}^2}{W_h^2}\right) \left(\frac{\partial u_2}{\partial t}\right)_m - \frac{4u_2 v_2}{R} W_{12}^2 + \frac{W_{12}^2}{W_h^2} A \quad (28)$$

6.2-2 Shock Fitting.

When the integration is carried out by the method of Section 6.4 in Lagrange coordinates it is possible ⁽⁵⁾ to carry the integration across the

(5)

First pointed out by von Neumann.

shock as if the motion were continuous, and it will be shown in Section 6.5 that this is a justifiable approximation if the shock is not too strong. Even, however, when the approximation should be sufficiently good this process introduces superponent oscillations which tend to obscure the detailed structure of the fluid motion behind the shock and which also make more difficult the detection of errors.

Accordingly, methods of "shock fitting" have been developed in which the shock conditions are satisfied correctly and the path of the shock is

fitted on to the boundary of the field of "regular" integration by means of certain subsidiary calculations made for each instant of time at which the integration is performed. The most satisfactory method devised for doing this is based on the following principle. It is assumed that the variation of all quantities between the shock and the edge of the field of integration is small and may be assumed linear in any space variable. If then at any time the value of the pressure, say, be known both at the shock and the edge, the pressure gradient at the shock may be deduced (assumed equal to the average gradient over the interval); similarly for any other space-gradient. When these values are substituted into one of the formulae of Equation (14) we can deduce the 'acceleration' of the shock and find the pressure behind it at a subsequent time. At the same time, we use the knowledge of conditions at the shock to extend the field of integration out from its bounding characteristic, and the cycle of operations may then be repeated at the next instant of time.

Consider the important case when the fluid ahead of the shock is at rest at constant pressure. Then, in the notation of Section 6.2-1, $X_1 = 0$, $A = 0$. If we use the Equation (27) for X_2 we find that behind the shock

$$\frac{dv_2}{dt} = \frac{2}{3 + (W_{12}^2/W_{12}^2)} \left\{ W_{12} \left(v \frac{\partial v}{\partial R} \right)_2 + \frac{1}{W_{12}} \left(v \frac{\partial p}{\partial R} \right)_2 + \frac{2u_2 v_2}{3} \right\} \quad (29)$$

In this case p_2 is a known function of v_2 , and therefore so also are u_2 , W_{12} , W_n ; that is, all the coefficients in Equation (29) are known functions of v_2 . The motion of the shock is given by the equation

$$\frac{dR}{dt} = v_1 W_{12} \quad (30)$$

Suppose at one time the values of $R, v = v_2$ are known at the shock. The gradients $(v \partial v / \partial R)$, $(v \partial p / \partial R)$ are calculated by taking the difference of v_2, p_2 with the adjacent values calculated in the integration, respectively.

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and dividing by the spatial interval. Then Equation (29) will determine dv_2/dt and (30) gives dr/dt ; thus are found the values of R , v at the shock at the next instant. Finally, the field is extended to complete the cycle by using the pressure gradient calculated here to find the acceleration of the particle at the edge of the field which is not otherwise determined by the integration behind the shock. In application, the Equations (29) and (30) are integrated to second order accuracy, rather than to first order as described above for simplicity of explanation, by determining v_2 by trial and error so that (29) integrates "backwards" correct to second order. The numerical value actually used will be discussed in Section 6.4 in connection with the integration.

As time increases, the gap between shock and the adjacent particle will increase, and we must do more than just extend the field of integration to this particle. This point is met by adding new particle-points in the gap by suitable interpolation when the gap becomes too large.

When the fluid ahead of the shock is in motion, the principle is exactly the same but the application is more tedious, because the pressure p_2 is no longer a function of the single variable v_2 but depends also on the varying quantities p_1 , v_1 . In the first place $X_1 \neq 0$ and has to be calculated at each step as follows. Suppose that the solution ahead of the shock is known and that for some time t_0 the values of R , u_1 , p_1 , v_1 , u_2 , p_2 , v_2 are known. Then analogously to (30) the shock velocity

$$\frac{dR}{dt} = v_1 W_{12} + u_1 \quad (31)$$

is known, and with it the position of the shock at the next instant. For this new position and time u_1 , p_1 , v_1 are already known and by differentiating them with their values at a suitable earlier time we can deduce the values of du_1/dt ... at time t_0 . Then X_1 may be calculated according to formula (22).

Next, since we do not know w_h^2 at t_2 , we cannot use Equation (20); instead we use Equation (24), putting $X_2 = X_1$.

$$\frac{dv_2}{dt} = \frac{2}{3+(w_2^2/w_{12}^2)} \left[w_{12} \left(1 + \frac{w_2^2}{2w_{12}^2}\right) \left(\frac{v}{\partial t}\right)_2 + \frac{3}{2w_{12}} \left(\frac{v}{\partial R}\right) + \frac{2u_2 v_2}{R} + \frac{X_1}{w_{12}^2} \right] \quad (32)$$

We have calculated X_1 , and w_2^2 is a known function of p_2, v_2 . Therefore, dv_2/dt may be evaluated and the cycle of operations completed just as before; only when we have found v_2, v_1, p_1 , at the next instant we have to calculate p_2 from the energy formula (14). The operations can be made correct to the second order as before, but with correspondingly more effort.

In application it may be more convenient to perform the integration simultaneously on both sides of the shock, although of course at each step we must integrate ahead of the shock first. This latter integration can be made by using the ordinary equations over the gap between the shock and the edge of the field; no additional information is needed because the shock runs into the characteristics ahead of the shock.

6.2-3 Shock Crossing an Interface.

When a shock-wave crosses an interface between two different media, a disturbance will, in general, be reflected back into the first medium and there will be a sudden change of pressure behind the shock. These rapid changes over short distances cannot be handled very satisfactorily by the integration process. If the shock is being treated by the approximate method described in section 6.5 this does not matter much, but if the shock is being treated as a discontinuity by a process such as that described in the last section, undesirable fluctuation will be introduced unless some way is used of getting away from the region of very rapid change.

The method adopted has been to use an analytic expansion for times and positions close to the instant the shock crosses the interface, and this will now be described. We will suppose that a shock is reflected back into the first medium; then the adjacent portion of the (R, t) plane

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may be divided into five sectors as shown in Figure 3.

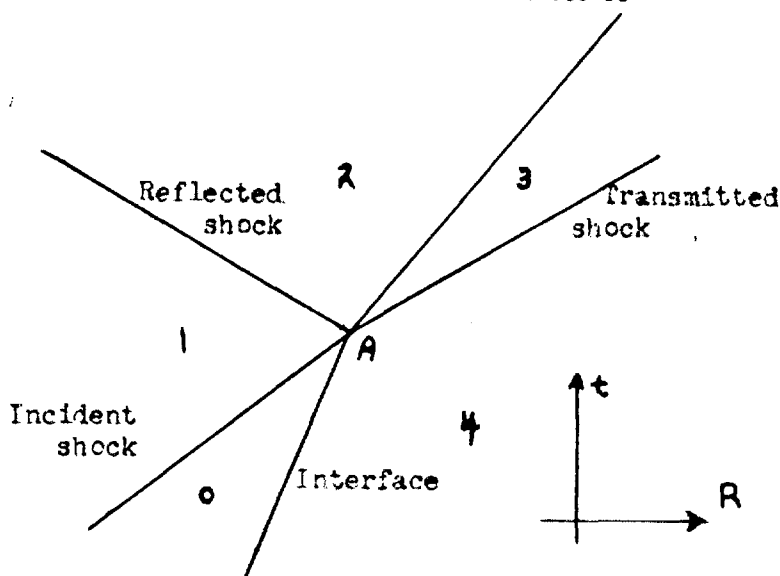


Figure 3

Region 0 is that ahead of the incident shock, 1 is behind the incident and ahead of the reflected shock. 2 and 3 are the regions in the two media between the reflected and transmitted shocks, and 4 is ahead of the transmitted shock. The solution will be known in 0,1,4; now the problem is to find an analytic expansion for regions 2 and 3.

Since pressure and velocity are continuous across the interface, it will be convenient to determine first the values of $p, u, \left(\frac{\partial p}{\partial t}\right)_m, \left(\frac{\partial u}{\partial t}\right)_m$ at the interface. When these have been found, it is easy to determine the values of all other quantities and their derivatives from the hydrodynamical equations in the two regions.

First, to determine p, u we must use the Equations (14) and (15) across the reflected and transmitted shocks. Since $u_1, p_1, v_1, u_4, p_4, v_4$ are known these will determine two relations between the values of p, u at the interface. As p_0 increases so does u_0 and the relation between p, u so determined may be represented by the curve T in the Figure 4. Similarly a curve R is determined by the reflected shock which has negative slope

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in the (p,u) plane. The lowest point on the curve R is (p_1, u_1) when the reflected shock just vanishes. If (p_1, u_1) lies above the curve T there is a rarefaction reflected, not a shock, and this case is discussed in the next subsection. When an intersection exists, its position may first be found approximately from this graphical picture and then by analytic approximation.

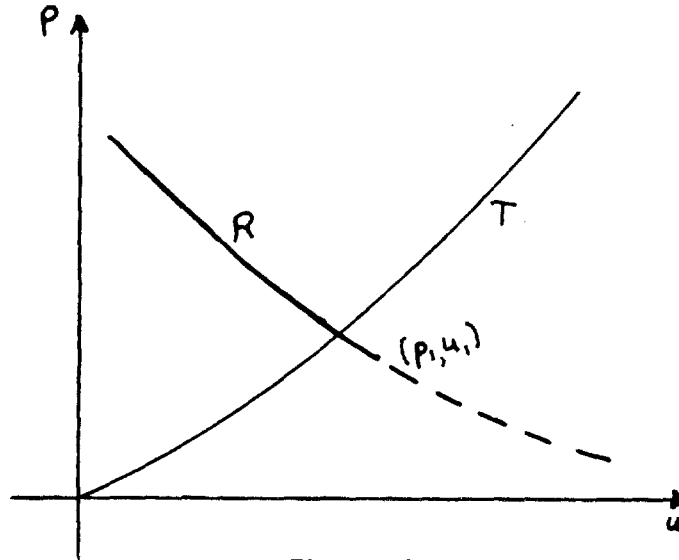


Figure 4

When $p_2 = p_3$, $u_2 = u_3$ and therefore v_2, v_3, \dots have been found, we can calculate $(\partial p / \partial t)$, $(\partial u / \partial t)$ by use of the formulae of Section 6.2-1. This requires the solution of the two simultaneous linear equations,

$$\begin{aligned} X_2 &= X_1 \\ X_3 &= X_4 \end{aligned} \tag{33}$$

Here X_1, X_4 are known now that the initial shock velocities have been found, and X_2, X_3 are taken in the form of Equation (28) wherein the only unknowns now are $(\partial p / \partial t), (\partial u / \partial t)$. W_1^2, A are calculated from the derived form of Equation (14).

6.2-4 Reflected Rarefaction Wave

If, in the (p,u) diagram of the last subsection (Figure 4) the point (p_1, u_1) lies above the curve T , then a rarefaction wave is reflected back into the first medium. The regions 1, 2 of Figure 3 are not separated now by a line of discontinuity but by a finite region F covered

by the rarefaction wave, as shown in Figure 5.

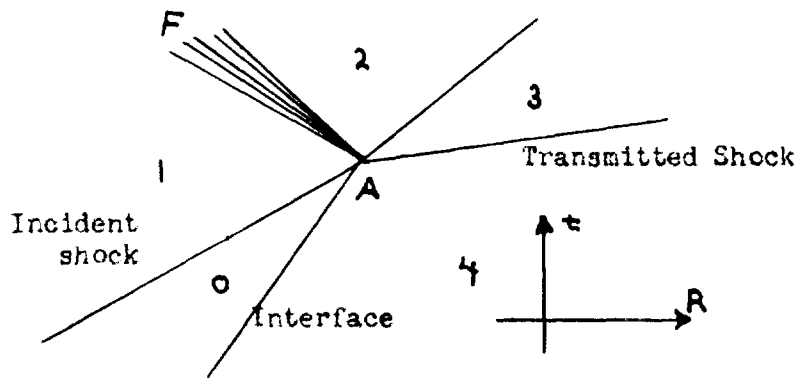


Figure 5

The boundaries of regions F and 1 and F and 2 are characteristics, having initially the slopes $(u_1 - c_1)$ and $(u_2 - c_2)$, respectively, and all the characteristics of this system in F pass through the apex A.

The condition that determines u_2, p_2 and provides the continuation downwards of the curve R in Figure 4, is

$$u_2 + \sigma_2 = u_1 + \sigma_1 \quad (34)$$

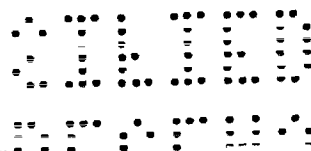
where σ is Riemann's function (see section 6.1-3) taken at the entropy S , which is unchanged through F.

$$\sigma = \int_V (\rho c) dv = \int_V (-\partial p / \partial v)_S^{1/2} dv \quad (35)$$

When u_2, p_2, v_2 have been determined we may determine $(\partial u / \partial t), (\partial p / \partial t)$ at the interface in a way similar to that used when there is a reflected shock. The Equations (33) are replaced by

$$\begin{aligned} Y_2 &= Y_1 \\ X_3 &= X_4 \end{aligned} \quad (36)$$

Here Y is a certain function of the derivatives of u, p, that is conserved across F, just as X is conserved across a shock. The expression for Y may be written as





$$Y = Z + 1/3 \left(v \frac{\partial S}{\partial r} \right) \int_v \left[\frac{\partial}{\partial S} \left(\rho_0 \right)^{3/2} \right] dv - \frac{1}{2t} \int_v \left[(c-\sigma) + (u+\sigma) \right] (\rho_0)^{1/2} dv \quad (37)$$

where $(u+\sigma)$ is a constant equal to the value of either side of Equation (34) and the upper limits of the integrals are arbitrary. $(v \partial S / \partial R)$ has equal values in regions 1,2 because the entropy is conserved and Z contains the velocity and pressure gradients,

$$Z = 1/\sqrt{\rho_0} \left[\left(\frac{\partial u}{\partial t} \right)_m + \left(1/\rho_0 \right) \left(\frac{\partial p}{\partial t} \right)_m \right] \quad (38)$$

$$= -\sqrt{c/\rho} \left[\frac{\partial u}{\partial R} + \left(1/\rho_0 \right) \left(\frac{\partial p}{\partial R} \right) + 2u/R \right] \quad (39)$$

This case is then just the same as in Section 6.2-3 except that a special treatment is needed to find the analytic expansion for the region F. If r is a Lagrangean coordinate as in Section 6.1-1 and $r = a$ at the apex A, then it is convenient to introduce a variable z defined by

$$z = (a-r)/t \quad (40)$$

where t is measured from zero at A. Then in F the analytic expansion can be written

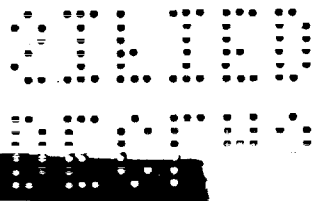
$$R(r,t) = a - t \phi_1(z) + 1/2 t^2 \phi_2(z) \quad (41)$$

The expansions for $\phi_1(z)$, $\phi_2(z)$ are most conveniently expressed in terms of a parameter μ , related to z by the equation

$$\rho_0 z^2 = -\left(\frac{\partial p}{\partial v} \right)_{v=\mu} \quad (42)$$

Then we find

$$\phi_1(z) = (c+\sigma)_{v=\mu} - (u+\sigma) \quad (43)$$



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and

$$\begin{aligned} \phi_z(z) = & 2(H\sqrt{\rho c})_{\mu, S_1} + (v\partial S/\partial R)(\partial p/\partial S)_{\mu, S_1} + \\ & 2/a \left[c^2 \left(\frac{\rho}{\rho_0} - 1 \right) + 2c(\bar{u} + \sigma - \sigma) \right]_{\mu, S_1} \end{aligned} \quad (44)$$

Here $H(v)$ is defined by the equation

$$Y(v) = Y(v_1) = Y_1 \quad (45)$$

6.5 INTEGRATION ALONG CHARACTERISTICS (Skyrme)

As has been stated in Section 6.1-4, the generalization of the Riemann method of integration to three-dimensional problems does not lead to a very satisfactory method of integration. Nevertheless, when mechanized calculation is not available, it seems the easiest to use. For this reason we shall describe in some detail the handling of the equations.

In the three-dimensional case Equation (10) contains an additional term, becoming

$$\begin{aligned} \partial u/\partial t + (u+c)\partial u/\partial R + c/\rho \left[(\partial \rho/\partial t) + u(\partial \rho/\partial R) \right] \\ + 1/\rho(\partial p/\partial R) + 2uc/R = 0 \end{aligned} \quad (46)$$

Now the pressure is a function of the density ρ and the entropy. In the most usual type of problem the entropy of a particle is constant throughout the motion⁽⁶⁾ and, therefore, if we differentiate along a streamline

$$\partial \rho/\partial t + u(\partial \rho/\partial R) = c^2(\partial \rho/\partial t + u\partial \rho/\partial R) \quad (47)$$

(6)

If the entropy were a function of the time only, we could transform the term $1/\rho(\partial p/\partial R)$ into $c^2/\rho(\partial \rho/\partial R)$ and derive similar equations; in the most general case when the entropy varies both in time and space, an additional term has to be added to the equations.

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Equation (46) may therefore be written,

$$(du/dt)_+ + 1/\rho c (dp/dt)_+ = -2uc/R \quad (48)$$

Where $(d/dt)_+$ denotes differentiation along a + characteristic, so that

$$(dR/dt)_+ = u + c \quad (49)$$

Two similar equations may be derived by changing the sign of c , namely

$$(du/dt)_- - 1/\rho c (dp/dt)_- = 2uc/R \quad (50)$$

and

$$(dR/dt)_- = u - c \quad (51)$$

These last four equations (48) - (51), on which the integration is based, may be handled by two different ways. In the former, we regard t as an independent variable and follow the characteristics at successive values of t . This is discussed further in Section 6.3-2.

Alternately we may regard these equations as a set of four simultaneous equations for R, t, u, p as functions of two parameters labeling the characteristics. If we solve the equations from this point of view we shall obtain a number of corresponding sets of values of the four variables. This is described in Section 6.3-3.

If we do not require a very detailed picture of the fluid motion, the second method is preferable, as it usually allows rather larger intervals to be taken. However, a detailed picture of, for example, the pressure distribution at each instant can only be found from this method of solution by subsequent interpolation; in such cases the first method would be better suited to the problem.

6.3-1 Transformation of the Equations.

Before changing the above equations into difference equations for the numerical integration, it is often desirable to transform them slightly. Equations (49) and (51) for the paths of the characteristics cannot profitably

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be altered, but the other two may be transformed along one of the following lines.

First, in the special case when the entropy is constant and p is a unique function of ρ , one may introduce Riemann's function σ instead of p as dependent variable

$$\sigma = \int^p dp/\rho c \quad (52)$$

and then (49) or (50) become

$$d(u \pm \sigma)/dt = \mp 2uc/R \quad (53)$$

Even when the pressure is not a unique function of density, it may be desirable to introduce some function $f(p)$ such that $(\rho c)(df/dp)$ is more nearly constant than ρc . In most physical problems the value of $\gamma = p/\rho c^2$ is nearly constant. This suggests that we divide the equations through by c and introduce $\log p$ as dependent variable.

$$1/c(du/dt)_{\pm} \pm p/\rho c^2(d \log p/dt)_{\pm} = \mp 2u/R \quad (54)$$

This form is useful if c does not vary widely over the intervals desired. On the right-hand side of both these last equations we may replace u/R by use of the equations of the characteristic paths,

$$u/R = \frac{u}{(u \pm c)} \left(d \log R/dt \right)_{\pm} \quad (55)$$

In some such way we shall transform these equations into a form

$$A(du/dt)_{\pm} \pm B(d f(p)/dt)_{\pm} = \mp C = \mp D(d \log R/dt)_{\pm} \quad (56)$$

such that the coefficients A , B and C or D vary as little as possible over the intervals desirable. If this equation be integrated over an interval Δt along the \pm characteristic we shall obtain

$$\bar{A}(\Delta u) \pm \bar{B}(\Delta f(p)) = \mp \bar{C}(\Delta t) = \mp \bar{D}(\Delta \log R) \quad (57)$$

where Δf denotes the change in the value of f over this interval and \bar{A} , \bar{B} ... denote certain average values of these coefficients.

When we use (57) as a difference equation, these averages must be replaced

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by a combination of values of the coefficients. If we use small intervals, then first-order accuracy will be sufficient and we can replace the average by the initial values in the interval. Generally, however, it will be profitable to use a formula correct to second order so that larger intervals may be taken. If by iteration or some other method we can obtain an approximate value of the coefficients at the far end of the interval, then second-order accuracy will be attained by the use of the arithmetic mean for the average. Accuracy of higher order could be reached only by the use of much more complex formulae.

The same considerations apply to the other two equations which will give on integration

$$\Delta R = (\bar{u} \pm c) \Delta t \quad (58)$$

and the average signal velocity may be replaced by its initial or arithmetic mean value as with the other equations.

6.3-2 First Method of Integration.

(1) Regular Integration

Suppose, as in Section 6.1-2, that we know the values of velocity, pressure, entropy within a range $R_1 \leq R \leq R_2$ at time t_0 . We take a set of points P_i evenly spaced (not necessarily at equal intervals of R) in this interval, between any two of which the hydrodynamical variables change little.

Through each point P_i will pass \pm characteristics having slopes $u \pm c$, which latter are calculable from the given initial conditions. If we now select a later time $t_1 = t_0 + \Delta t$ then in first approximation these characteristics will pass through points Q_i^{\pm} in the (R, t) plane where, according to (58),

$$R(Q_i^{\pm}) = R(P_i) + (u \pm c)_{P_i} (\Delta t) \quad (59)$$

Also if we integrate along these characteristics to first order we can find the radius of $A_1 u \pm B_1$ at Q_i^{\pm} respectively. Thus, from (57)

$$A_i u \pm B_i f(p) = A_i u_i \pm B_i f(p_i) \quad (60)$$

where, for brevity, A_i denotes the value of A at P_i , etc. Suppose now the point Q_i^+ lie between Q_j^- and Q_{j+1}^- ,

$$R(Q_j^-) \leq R(Q_i^+) \leq R(Q_{j+1}^-) \quad (61)$$

Then we use linear interpolation over this interval to determine the value of $Au - Bf(p)$ at Q_i^+ (A, B have values averaged between those at the ends of the interval). If this is combined with the value of $A_i u + B_i f(p)$ determined from (60), we can find the values of $u, f(p)$ separately at the point Q_i^+ . We also need to know the value of the entropy at Q_i^+ . By hypothesis the entropy is a known function of the particle label-coordinate. This is found by integration of one of the equations (9)

$$(dm/dt)_\pm = 3\rho_0 r^2 (dr/dt)_\pm = \pm 3R^2(\rho c) \quad (62)$$

(This is treated as a difference equation exactly as in Equation (58).)

Now that we have determined the values of all variables at the points Q_i^\pm (the end points may have to be treated specially as in (2) below) we can calculate the values of A, B, \dots there at, and then repeat the integration to second-order accuracy by using arithmetic means for the average in the difference formulae. In subsequent steps of the integration it will not be necessary to carry out the integration twice; it will be sufficient to use values of A, B, \dots at the far ends of the intervals determined by extrapolation along the paths of the characteristics and carry out the second-order integration immediately.

(2) Boundaries

Consider for example an interface between two different media. First we must follow the path of the interface from step to step just as we follow the path of a characteristic, using the equation

$$(dr/dt)_{\text{interface}} = u \quad (63)$$

The \rightarrow characteristics will run into the interface from the left (smaller values of R) and the \leftarrow characteristics from the right. So then at the new time t_1 , when we have found the position R of the interface, we extrapolate the values of $Au+Bf(p)$ from the left and $Au-Bf(p)$ from the right to this interface point and then solve for $u, f(p)$ at this point as usual (the values of A, B and the form of $f(p)$ may, of course, be quite different on the two sides of the interface). The only problem remaining is that of the continuation of characteristics that cross the interface; either we may interpolate to find the time at which the signal crosses the interface and the new value of the slope of the characteristics and then treat this characteristic specially for the subsequent interval (because the time interval is not the normal one), or we may drop the characteristic when it crosses the interface and introduce a new one on the appropriate side starting from the interface at one of the chosen times t_1 .

The progress of a shock boundary is treated similarly. The shock path is found by integration of

$$(dR/dt)_{\text{shock}} = U \quad (64)$$

where U , the shock velocity, is a function of the known conditions ahead and any one variable behind the shock. The value of $Au+Bf(p)$ extrapolated from the left gives a relation between u, p at the shock which determines u, p separately by combination with the shock conditions. This all assumes that the solution has been found ahead of the shock, and this can always be done as explained in the last section; in practice it may be convenient to perform the integration simultaneously on both sides of the shock.

6.3-3 Second Method of Integration.

(1) Regular Integration

Suppose, as before, that we are given initial values in an interval

$R_1 \leq R \leq R_2$ at time t_0 . Then in just the same way we can find the initial slope of the characteristics through a set of points P_1 . Instead, however, of finding the points where these paths cross a line of fixed time t_1 in the (R,t) plane, we find the points Q_1 of intersection of adjacent characteristics of opposite systems. Then, to first order, the values of R, t at such a point Q_1 will be determined by solving the simultaneous equations

$$\left. \begin{aligned} R &= R(P_1) + (u+c)_{P_1} (t-t_{P_1}) \\ R &= R(P_{i+1}) + (u-c)_{P_{i+1}} (t-t_{P_{i+1}}) \end{aligned} \right\} \quad (65)$$

where in this case $t_{P_1} = t_{P_{i+1}} = t_0$. Next we find by use of Equation (60) (where Δt has now the value $(t-t_{P_1})$ or $(t-t_{P_{i+1}})$), the values of $A_i u + B_i f(p)$ and $A_{i+1} u - B_{i+1} f(p)$ at the (same) point Q_1 , and these may then be solved for u, p . The entropy at Q_1 is found in the same way by integration of Equation (61) along either characteristic.

When this first-order integration has been completed, the second approximation can be carried out in just the same way, using the first-order values at Q_1 to find the mean values of A, B, \dots over the intervals. In the subsequent integration we again use an extrapolation process to determine approximate values of A, B, \dots at Q_1 . However, in this method it is not convenient to extrapolate along the characteristics (because the intervals between points determined may be irregular in any reasonable variable). The simplest method seems to be the use of linear interpolation over a quadrangle in the (R,t) plane bounded by characteristics. Thus, if the next points determined on the \pm characteristics through a point P are Q, R respectively, and we seek now the values of the variables at the intersection S of the other characteristics through Q, R (See Figure 6), then as first approximation to the value f_S of any quantity f at S we assume

$$f_S = f_Q + f_R - f_P \quad (66)$$

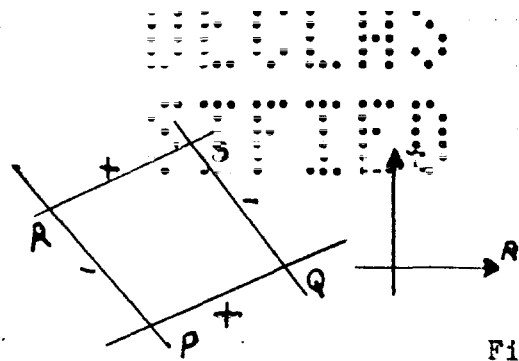


Figure 6.

It has been found convenient in some cases, where the variations of material velocity u are greater than those of sound velocity c , to proceed by assuming a value of u at S (in first approximation given by (66)), and correcting this until the values of the pressure determined by integration along either characteristic become equal.

(2) Boundaries

The treatment of interfaces and shock boundaries is rather troublesome by this method. Since we cannot carry characteristics across an interface in one step we must always arrange that one of our intersection points Q_i lie at the interface whenever a characteristic crosses it. Suppose that the point P of Figure 7 lies on the interface and that the $+$ characteristic RS crosses the interface before QS .

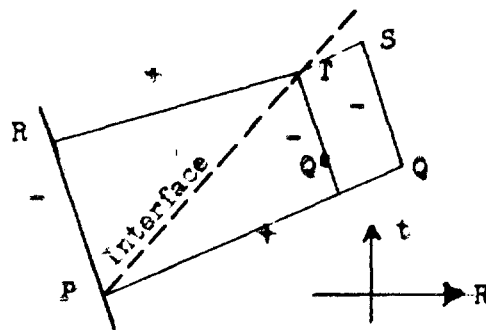


Figure 7

The position of the intersection T of this characteristic with the interface may be determined as for the intersection of two characteristics: next we have to determine a point Q' on the $+$ characteristic PQ such that the $-$ characteristic through Q' pass also through T . The point T may then be treated as an intersection of characteristics through R, Q' in the usual way. The procedure

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is tedious because it may be necessary to change the position of Q' when going to second approximation. The interpolation formulae for finding position Q' and the values of the variables thereat can easily be obtained from the formulae used in Section 6.3-3(1)

Shock boundaries are rather easier to handle. Suppose that in the Figure 7 P lies on the shock and that PT is the path of the shock. Suppose we assume a value of the shock velocity U at T ; then the material velocity and sound velocity are determined simultaneously. We can now determine the position of T in the usual way (correct to second-order) and integration along RT gives a relation between u, p that must be satisfied at T . The value of U assumed must then be corrected so that this relation is true at T .

6.4 NUMERICAL SOLUTION OF THE HYDRODYNAMICAL EQUATIONS ON I.B.M. MACHINES (Nelson)

6.4-1 Analytic Form of the Equations.

In the preceding sections of this chapter, the hydrodynamical equation and methods for its solution are discussed. The numerical methods get the solution by integrating step-by-step, from one interval to the next. In each integration step they involve an appreciable number of elementary calculations. If a detailed picture of the fluid motion is required, small intervals must be used; then there will be a large number of integration steps and an enormous number of elementary operations--of the order of a few hundred thousand. Such a large number of operations makes the doing of even a single problem on an ordinary calculation machine almost prohibitive. If several problems are to be solved, it becomes necessary to thoroughly mechanize the method of solution. In this section a method is described in which the routine operations are done on I.B.M. machines.

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The Lagrangean representation described in 6.1-1 is the most convenient form of the hydrodynamic equation to use in T. B. M. machine solution. It is a partial differential equation with two independent variables, r and t.

$$\frac{\partial^2 R}{\partial t^2} = -v_0 \frac{R^2}{r^2} \frac{\partial p}{\partial r} = -3v_0 R^2 \frac{\partial p}{\partial r^3} \quad (67)$$

Here as in Section 6.3 the problem is restricted to the case of spherical symmetry. The coordinate r identifies a spherical shell of material, it is the radius of the spherical shell when the material is in a standard configuration of uniform density, $\frac{1}{v_0}$. R is the actual radius at time t of this spherical shell. p is the pressure. It is a known function, the equation of state, of the specific volume, v, and of the entropy S. Also, we have

$$v = v_0 \frac{\partial R^3}{\partial r^3} \quad (68)$$

Conduction of heat is neglected; therefore, so long as the motion is continuous, the entropy of a material particle does not change, $\frac{\partial S}{\partial t} = 0$. What happens at a discontinuity is discussed in Section 6.4-5.

6.4-2 Difference Form of the Equations.

A solution to the problem is the obtaining of the actual radius R, of the spherical shells identified by the coordinate r for all times t, of interest. In the numerical solution, R is calculated for a discrete set of values of r and t. These values of r are labeled by an index i, which will be used as a subscript; the values of t are labeled by an index n, which will be used as a superscript. Thus the radius of spherical shell i at time n is R_i^n . The derivatives in Equations (67) and (68) are approximated as finite difference expressions.

$$\frac{\partial^2 R}{\partial t^2} \longrightarrow \frac{R_i^{n+1} - 2R_i^n + R_i^{n-1}}{(\Delta t)^2} \quad (69)$$

$$\frac{\partial R^3}{\partial r^3} \longrightarrow \frac{(R_i^n)^3 - (R_{i-1}^n)^3}{\Delta r^3} \quad (70)$$

$$\Delta t \equiv t^{n+1} - t^n$$

$$\Delta r^3 \equiv r_i^3 - r_{i-1}^3$$

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The partial differential equation then becomes a finite difference equation,

$$\frac{R_i^{n+1} - 2R_i^n + R_i^{n-1}}{(\Delta t)^2} = -\frac{v_o(R_i^n)^2}{r_i^2} \left(\frac{p_{i+\frac{1}{2}}^n - p_{i-\frac{1}{2}}^n}{\Delta r} \right)$$

or

$$R_i^{n+1} = 2R_i^n - R_i^{n-1} + \frac{v_o(\Delta t)^2 (R_i^n)^2}{r_i^2 \Delta r} \left(p_{i+\frac{1}{2}}^n - p_{i-\frac{1}{2}}^n \right) \tag{71}$$

$$p_{i-\frac{1}{2}}^n = p(v_{i-\frac{1}{2}}^n, S_{i-\frac{1}{2}}) \tag{72}$$

$$v_{i-\frac{1}{2}}^n = v_o \frac{(R_i^n)^3 - (R_{i-1}^n)^3}{\Delta r^3} \tag{73}$$

The difference equation represents the differential equation exactly only in the limit as Δr and Δt go to zero. Since finite intervals are used in the numerical calculation, errors are made. These errors can be studied by expanding significant quantities in power series.

$$R_i = R_i^n + \left(\frac{\partial R}{\partial t} \right)_i^n (t-t^n) + \frac{1}{2} \left(\frac{\partial^2 R}{\partial t^2} \right)_i^n (t-t^n)^2 + \frac{1}{6} \left(\frac{\partial^3 R}{\partial t^3} \right)_i^n (t-t^n)^3 + \frac{1}{24} \left(\frac{\partial^4 R}{\partial t^4} \right)_i^n (t-t^n)^4$$

$$R_i^{n+1} = R_i^n + \left(\frac{\partial R}{\partial t} \right)_i^n \Delta t + \frac{1}{2} \left(\frac{\partial^2 R}{\partial t^2} \right)_i^n (\Delta t)^2 + \frac{1}{6} \left(\frac{\partial^3 R}{\partial t^3} \right)_i^n (\Delta t)^3 + \frac{1}{24} \left(\frac{\partial^4 R}{\partial t^4} \right)_i^n (\Delta t)^4$$

$$R_i^{n-1} = R_i^n - \left(\frac{\partial R}{\partial t} \right)_i^n \Delta t + \frac{1}{2} \left(\frac{\partial^2 R}{\partial t^2} \right)_i^n (\Delta t)^2 - \frac{1}{6} \left(\frac{\partial^3 R}{\partial t^3} \right)_i^n (\Delta t)^3 + \frac{1}{24} \left(\frac{\partial^4 R}{\partial t^4} \right)_i^n (\Delta t)^4$$

$$\frac{R_i^{n+1} - 2R_i^n + R_i^{n-1}}{(\Delta t)^2} = \left(\frac{\partial^2 R}{\partial t^2} \right)_i^n + \frac{1}{12} \left(\frac{\partial^4 R}{\partial t^4} \right)_i^n (\Delta t)^2 + \dots$$

Thus the difference equation (69) represents $\frac{\partial^2 R}{\partial t^2}$ evaluated at time n and point i with an error proportional to $\frac{(\Delta t)^2}{12}$. If it were used to represent $\left(\frac{\partial^2 R}{\partial t^2} \right)_i$ at any other point within the interval $n + \frac{1}{2}$ and $n - \frac{1}{2}$, the error would contain

$\begin{matrix} \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{matrix}$

terms proportional to Δt . This evaluation of the derivative at the midpoint of the interval over which the differences are taken is called a central difference. In the absence of specific information concerning the higher derivatives of a function, it is best. For this reason the specific volume obtained by the differencing process in Equation (73) is labeled $v_{i-\frac{1}{2}}^n$. $i-\frac{1}{2}$ is the midpoint of the interval between i and $i-1$.

Similarly, the other derivative in Equation (67) has the expansion

$$\left(\frac{\partial p}{\partial r^3}\right)_i^n = \frac{p_{i+\frac{1}{2}}^n - p_{i-\frac{1}{2}}^n}{\Delta r^3} - \frac{1}{24} \left(\frac{\partial^3 p}{\partial (r^3)^3}\right)_i^n (\Delta r^3)^2 + \dots$$

This equation gives the error in $\frac{\partial p}{\partial r^3}$ as calculated from a set of known values of p . But in the actual numerical solution, p is calculated from v and S , which may themselves be in error. The entropy, S , will here be considered as known with arbitrary accuracy since it is obtained in a procedure independent of this set of difference equations. v is calculated from a difference Equation (75), which has an error

$$-\frac{v_0}{24} \left(\frac{\partial^2 v}{\partial (r^3)^2}\right)_{i-\frac{1}{2}}^n (\Delta r^3)^2$$

If the above expression for $\frac{\partial p}{\partial r^3}$ is modified to include this effect it becomes

$$\left(\frac{\partial p}{\partial r^3}\right)_i^n = \frac{p_{i+\frac{1}{2}}^n - p_{i-\frac{1}{2}}^n}{\Delta r^3} - \frac{(\Delta r^3)^2}{24} \left[\frac{\partial^3 p}{\partial (r^3)^3} + \frac{\partial^2 p}{\partial r^3 \partial v} \frac{\partial^2 v}{\partial (r^3)^2} + \frac{\partial p}{\partial v} \frac{\partial^3 v}{\partial (r^3)^3} \right]_i^n$$

Here $p_{i+\frac{1}{2}}^n$ and $p_{i-\frac{1}{2}}^n$ are interpreted as calculated from $v_{i+\frac{1}{2}}^n$ and $v_{i-\frac{1}{2}}^n$, which are calculated from Equation (73). It has been assumed that the intervals $i + \frac{1}{2}$ and $i, i-1$ have the same Δr^3 .

The procedure in the solution is to calculate R_i^{n+1} from data at times n and $n-1$. If this data is assumed to be correct, R_i^{n+1} will be in error, owing to the finite size of the intervals, by the following amount:

$$\frac{(\Delta t)^2}{12} \left(\frac{\partial^4 H}{\partial t^4}\right) - \frac{(\Delta r^3)^2}{24} \left[\left(\frac{\partial^3 p}{\partial (r^3)^3} + \frac{\partial^2 p}{\partial r^3 \partial v} \frac{\partial^2 v}{\partial (r^3)^2} + \frac{\partial p}{\partial v} \frac{\partial^3 v}{\partial (r^3)^3}\right) \right] \quad (74)$$

This error will be small if Δt and Δr^3 are small or if the compressions



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in the material are nearly constant.

6.4-3 Size of Intervals and Stability of the Solution.

The intervals in r and t must be chosen small enough to make the error term (74) negligible. In r this means that there must be enough points to give a good definition of p . The number of points needed in a given section of material may change during the course of a problem, for the pressure distribution may change radically in that time. How the intervals should be distributed in r will depend on the expected pressure distribution. If the pressure is approximately a linear function of the mass of material, as is the case in the early stages of a blast wave in air, the intervals are best chosen equally spaced in r^3 . Then, too, the expected errors will be the least in the central difference formulas. In other problems p is a slowly varying function of r and a rapidly varying function of r^3 . There it is better to use intervals equally spaced in r itself. Then central difference accuracy could be maintained if v were calculated by the following formula instead of (73),

$$v_{i-\frac{1}{2}}^n = v_0 \left(\frac{R_{i-\frac{1}{2}}^n}{r_{i-\frac{1}{2}}} \right)^2 \frac{R_i^n - R_{i-1}^n}{\Delta r}$$

However, the use of this formula would greatly complicate the procedure.

After the intervals in r are chosen, Δt cannot be chosen independently. The discussion of characteristics in Section 6.1-2 predicts Δt should be chosen so that R_i^{n+1} lies within the domain bounded by the characteristics through R_{i+1}^n and R_{i-1}^n . This means that Δt should be less than $\left(\frac{r}{R}\right)^2 \frac{\Delta r}{v_0 \sqrt{-\frac{\partial p}{\partial v}}}$. If Δt is larger than this quantity, R_i^{n+1} cannot correctly be obtained from information within the interval $i+1$ and $i-1$; at time n , that is, the situation outside of this interval influences the value of R_i^{n+1} .

This same condition on Δt can be derived directly from the difference Equation (71). The question is put in the following manner: If an error δ is made in R_i^n , what error does it produce in R_{i-1}^{n+1} and R_{i+1}^{n+1} ?

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Let R_1^n be its correct value and $R_1^n + \delta$ its wrong value. Then the specific volumes $v_{i-\frac{1}{2}}^n$ and $v_{i+\frac{1}{2}}^n$ calculated will differ from the correct specific volumes..

$$v_{i-\frac{1}{2}}^n = \frac{v_0 [(R_1^n + \delta)^3 - (R_{i-1}^n)^3]}{\Delta r^3} = v_{i-\frac{1}{2}}^n + \frac{3\delta v_0 (R_1^n)^2}{\Delta r^3} + O(\delta^2)$$

$$v_{i+\frac{1}{2}}^n = v_{i+\frac{1}{2}}^n - \frac{3\delta v_0 (R_1^n)^2}{\Delta r^3} + O(\delta^2).$$

The corresponding calculated pressures are also in error.

$$p_{i-\frac{1}{2}}^n = p_{i-\frac{1}{2}}^n + \left(\frac{\partial p}{\partial v}\right)_{i-\frac{1}{2}}^n \left[\frac{3\delta v_0 (R_1^n)^2}{\Delta r^3} \right]$$

$$p_{i+\frac{1}{2}}^n = p_{i+\frac{1}{2}}^n - \left(\frac{\partial p}{\partial v}\right)_{i+\frac{1}{2}}^n \left[\frac{3\delta v_0 (R_1^n)^2}{\Delta r^3} \right]$$

If these quantities are substituted into (71), an incorrect value of the radius at time $n + 1$ will be calculated.

$$R_1^{n+1} = 2R_1^n + 2\delta - R_1^{n-1} + \frac{3v_0(\Delta t)^2}{\Delta r^3} \left[\frac{(R_1^n)^2 + 2\delta R_1^n}{2} \right] \left[p_{i-\frac{1}{2}}^n - p_{i+\frac{1}{2}}^n \right] + \frac{3\delta v_0 (R_1^n)^2}{\Delta r^3} \left(\frac{\left(\frac{\partial p}{\partial v}\right)_{i-\frac{1}{2}}^n}{2} + \frac{\left(\frac{\partial p}{\partial v}\right)_{i+\frac{1}{2}}^n}{2} \right)$$

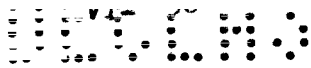
The correct formula for this radius is

$$R_1^{n+1} = 2R_1^n - R_1^{n-1} + \frac{3v_0(\Delta t)^2 (R_1^n)^2}{\Delta r^3} (p_{i-\frac{1}{2}}^n - p_{i+\frac{1}{2}}^n)$$

Hence the error is

$$R_1^{n+1} - R_1^{n+1} = 2\delta \left\{ 1 + \left[\frac{3v_0 \Delta t (R_1^n)^2}{\Delta r^3} \right]^2 \left[\frac{\left(\frac{\partial p}{\partial v}\right)_{i-\frac{1}{2}}^n + \left(\frac{\partial p}{\partial v}\right)_{i+\frac{1}{2}}^n}{2} \right] + 3v_0(\Delta t)^2 R_1^n \left(\frac{p_{i-\frac{1}{2}}^n - p_{i+\frac{1}{2}}^n}{\Delta r^3} \right) \right\}$$

The last term is just $\frac{R_1^{n+1} - 2R_1^n + R_1^{n-1}}{R_1^n}$ which for any reasonable choice



of Δt should be very small compared to Δx , so it can be neglected. The second term will be called δ . Thus, the error in R_i^{n+1} produced by an error δ in R_i^n is $2\delta(1-L)$. Similarly, the error in R_i^{n+1} produced by an error δ in R_i^{n-1} is $-\delta L$, by an error δ in R_{i-1}^n is $+\delta L$, and by an error δ in R_{i+1}^n is $+\delta L$. The propagation of these errors is shown in the following chart in which an error 1 was made in point i at cycle n . In constructing this chart it has been assumed that L does not vary significantly from one point to the next. This is true if the pressure does not change much in one interval. The error made in the radius of point i at time n spreads to other points. If $L > 1$, the error will spread one point per cycle. If $L < 1$, it will initially spread one point per cycle but quickly will become attenuated and move with the speed of sound.

	$i-2$	$i-1$	i	$i+1$	$i+2$
$n-1$	0	0	0	0	0
n	0	0	1	0	0
$n+1$	0	$+L$	$2(1-L)$	$+L$	0
$n+2$	L^2	$-4L^2+4L$	$6L^2-8L+3$	$-4L^2+4L$	L^2

The error in a given point oscillates in time. If $L > 1$, the amplitude of the oscillation will grow beyond bound. If $L < 1$, the amplitude of the oscillation will remain bounded. The sum of the errors in the radii of the points at any cycle is independent of L and is equal to the magnitude of the error times the number of cycles since the error was made.

In any calculation, one tries to have it free from mistakes. But there are errors which are inherent in any numerical computation. These are rounding errors, owing to the finite number of digits carried in each number.

If $L > 1$ rounding errors will introduce large and uncontrollable oscillations in the points. If $L < 1$, the oscillations from the rounding errors will remain small and ones from different points will interfere with each other. Therefore, in order to have a stable solution, the time



interval, Δt , must be chosen to make $L \ll 1$.

$$-\left(\frac{v_0 \Delta t R^2}{r^2 \Delta r}\right)^2 \left(\frac{\partial p}{\partial v}\right) < 1$$

or

$$\Delta t < \frac{r^2 \Delta r}{v_0 R^2 \sqrt{-\frac{\partial p}{\partial v}}} \quad (75)$$

This restriction means that if Δr is made small to secure spatial detail in the solution, Δt must be made correspondingly small.

6.4-4 Arrangement of the Computation Steps.

The difference equation (71) is the basis for the numerical work. It expresses the radius of a point at a time $n + 1$ in terms of its radius at times n and $n-1$ and the pressure distribution at time n . Equations (72) and (73) express the pressure at time n in terms of radii at time n . This suggests as a procedure of calculation to calculate from the radii at time n the pressure distribution at time n and then insert it into (71) for the calculation of the radii at time $n + 1$. This set of operations can be repeated to give the radii at time $n + 2$ and so on, giving rise to a cyclic procedure.

In Equation (72), the pressure p is given as a function of two variables, v and S . This function is usually so complicated that it is impractical to compute the pressure from v and S each time it is needed. If a table of p as a function of v and S is constructed, it would contain one entry for each pair of values of v and S . In most problems the range of v and S is so great and consequently, the number of table entries needed is so large, that this is also an impractical procedure. However, it has been found that many equations of state can be adequately approximated by a form which requires only a single entry table and a simple calculation. This form is

$$p = F_1 \frac{v}{a} + b F_2 \frac{v}{a} \quad (76)$$

where b and a are known functions of S . A practical table would have of the order of 1000 entries with one I.B.M. card for each value of $\frac{v}{a}$. Both F_1

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and F_2 and their first differences can be punched on the same card. A thousand entry table would contain entries for every possible value of a 3 digit $\frac{V}{a}$. In the problems we solved, we used a 5 digit $\frac{V}{a}$. Values of F_1 and F_2 and their first differences to the first 3 digits of $\frac{V}{a}$ were read out of a table, and the values of F_1 and F_2 corresponding to the 5 digit $\frac{V}{a}$ were obtained by linear interpolation.

One I.B.M. card is used to represent each material point. The collection of cards representing all the material points at a definite time n is called the deck belonging to cycle n . The computation of the radius at time n and the pressure distribution at time n is done on the deck of cards of cycle n .

The most efficient arrangement of the elementary operations within a cycle depends on the I.B.M. machines available. The procedure at Los Alamos was developed on the basis of triple product multipliers and the tabulator-summary punch combination (see Chapter 1). The triple product multipliers compute the expressions $A \times B \times C$ or $A \times (B \pm C)$ in one run of the cards through the machine. These machines reduced significantly the number of operations and the number of card columns needed in a cycle compared to an arrangement using ordinary multipliers. The tabulator-summary punch combination was used to list the data for cycle n , to difference a few quantities, and to transfer to a new deck of cards the data necessary for the computations in cycle $n + 1$.

Each I.B.M. card, which represents a definite material point, has punched on it the numbers necessary to perform the calculations for this point. Some of the quantities depend only on the coordinate r , or the index i , and hence for a given point, do not change in time. They are, in addition to the identification of the card, the quantities $\frac{v_0(\Delta t)^2}{r_i^2 \Delta r}$, $\frac{v_0}{a_{i-\frac{1}{2}}(\Delta r^3)_{i-\frac{1}{2}}}$, and $b_{i-\frac{1}{2}}$. They are called rates.

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At the start of cycle n , the following quantities are punched in card i , in addition to its identification and rates: R_i^{n-1} , $2R_i^{n-1} - R_i^{n-2}$, and $dp_i^{n-1} \equiv$

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$P_{i-\frac{1}{2}}^{n-1} - P_{i+\frac{1}{2}}^{n-1}$. The sign of dp is represented by an X-punch in an appropriate column. From this group of quantities, R_i^n can be calculated.

The computation is arranged in the following series of operations:

1) Triple multiplication: $\frac{v_0(\Delta t)^2}{r_i^2 \Delta r} (R_i^{n-1})^2$

2) Multiplication and addition:

$$R_i^n = (2R_i^{n-1} - R_i^{n-2}) + \frac{v_0(\Delta t)^2}{r_i^2 \Delta r} (R_i^{n-1})^2 dp_i^{n-1}$$

3) Triple multiplication: $(R_i^n)^3$

4) Transfer of R^3 of point $i-1$ to card i by the reproducer.

5) Addition and multiplication:

$$\left(\frac{v}{a}\right)_{i-\frac{1}{2}}^n = \frac{v_0}{a_{i-\frac{1}{2}}(\Delta r^3)_{i-\frac{1}{2}}} \left[(R_i^n)^3 - (R_{i-1})^3 \right]$$

6) Sort cards into ascending order on first 3 digits of $\frac{v}{a}$.

7) Merging in collator work cards with table cards bearing F_1 and F_2 .

8) Multiplication: Interpolate F_1 .

9) Multiplication: Interpolate F_2 .

10) Sort out table cards.

11) Multiplication and addition: $p_{i-\frac{1}{2}}^n = F_1 + b_{i-\frac{1}{2}} F_2$

12) Tabulator and Summary punch: List data from cycle n , transfer identification and rates to new deck in summary punch, compute $2R_i^n - R_i^{n-1}$ and dp_i^n and punch on new deck.

A detailed discussion of each operation is given in 6.4-7.

6.4-5 Boundary Conditions.

The set-up just described is a procedure for the calculation of R_i^{n+1} from R_i^n , R_{i+1}^n , and R_{i-1}^n , R_i^{n-1} : i.e., if the radii of all points are given at times n and $n-1$, the radii of these points are calculated at later times by successive application of the difference equation (71). But the initial conditions, the radii at times n and $n-1$, and the difference equation do not by

themselves correspond to a unique physical situation, and hence do not have a unique solution. They must be supplemented by other conditions, boundary conditions. The boundary conditions are conditions imposed at two material points, two values of r . They will be different for different physical problems. Here they will be described for a definite problem, a spherical blast wave in air.

One of the conditions is imposed at the center of the blast. The material point which was originally at the center remains there: i.e., the point with coordinate $r = 0$ has the same radius, $R = 0$ for all times. This condition is easily worked into the machine procedure. The radius of the point, $r = 0$, directly affects the calculation of other points only in the computation of v for the point with next larger r . Since in the calculation the cubes of the radii are subtracted from the cube of the radius of the first point with non-zero r , it is only necessary to have no I.B.M. card representing the point $r = 0$. Then the zero will automatically get transferred (in operation 4), as the radius cubed of the point $r = 0$, to the next card.

The other boundary condition is that there is an outgoing spherical shock wave. At this shock wave the pressure, density, and material velocity change discontinuously. The derivative of the pressure, $\frac{\partial p}{\partial r}$, does not exist across the shock; hence, the partial differential equation cannot be used to continue the solution across the shock front. Boundary conditions must be applied to connect the solution on one side with the solution on the other side. These boundary conditions, which are derived from conservation laws, are the Hugoniot relations discussed in 6.2-1.

The state of the system outside the shock wave is that the air is at rest at normal pressure, density and entropy. When the shock wave hits a particular spherical shell of air, it changes discontinuously its pressure from one atmosphere to a pressure p , and its density from normal density,

$\frac{1}{v_0}$, to a density $\frac{1}{v_s}$. Here the subscript s is used to identify a quantity evaluated at the shock on the high pressure side. In these discontinuous changes some energy is transformed into heat, giving rise to a change in entropy of the air. The shock moves with respect to the material; hence its position, r_s , is a function of the time. Since a point has not moved from its original position at the time the shock hit it, its actual radius R_s is the same as its label coordinate r_s , $R_s = r_s$, and r_s is a function of only one independent variable, the time, t .

The Hugoniot relations are:

velocity of the shock

$$\frac{d}{dt} r_s = v_0 W \quad (77)$$

$$W \equiv \sqrt{\frac{p_s - p_0}{v_0 - v_s}} \quad (78)$$

material velocity

$$u_s \equiv \left(\frac{\partial R}{\partial t} \right)_s = \sqrt{(p_s - p_0)(v_0 - v_s)} \quad (79)$$

the change in internal energy produced by the shock

$$E_s - E_0 = \frac{1}{2}(p_s - p_0)(v_0 - v_s) \quad (80)$$

The internal energy, E , and the pressure, p , are known functions of v and S . If these functions are substituted into (80) there results an equation relating the entropy in the shock to the specific volume in the shock v_s . This equation can be solved (numerically, if necessary) for the entropy in terms of v_s and this result substituted into the equation of state $p = p(v, S)$. The resultant function in v_s alone is called ψ .

$$p(v_s, S_s) = \psi(v_s) \quad (81)$$

If $\psi(v_s)$ is used in (78) and (79), S_0 has been eliminated from the necessary relations, which now become

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$$\frac{dr_s}{dt} = v_0 W \quad (82)$$

$$W(v_s) = \sqrt{\frac{\psi - p_0}{v_0 - v_s}} \quad (83)$$

$$u_s = \sqrt{(\psi - p_0)(v_0 - v_s)} \quad (84)$$

If the general solution of the partial differential equation were known, these Equations (82), (83), and (84) could be used to eliminate the arbitrary constants in it and to locate the position of the shock. The solution described here is a numerical solution and it is difficult to use these relations alone, if any sort of accuracy is needed. To supplement them then it has been convenient to derive from them expressions for $\frac{dv_s}{dt}$ and $\frac{d^2 r_s}{dt^2}$. (See 6.1-2).

These expressions are:

$$\frac{dv_s}{dt} = \left[\frac{4u_s v_s w}{r_s} - \frac{2v_0 W^{3/2}}{(3W + w)} \left(\frac{\partial v}{\partial r} \right)_s - 2v_0 \sqrt{W} \left(\frac{\partial p}{\partial r} \right)_s \right] \quad (85)$$

$$w = - \frac{d\psi}{dv} \quad (86)$$

$$\frac{d^2 r_s}{dt^2} = \frac{v_0}{2u_s} \frac{dv_s}{dt} (w^2 - W^2) \quad (87)$$

These formulas, the Hugoniot relations and their time derivatives, form a practical basis for fitting the boundary conditions at the shock front. The formula for $\frac{dv_s}{dt}$, (85), contains first space derivatives of p , v . In that respect, it is of the same order as the partial differential equation. Here, however, it is not possible to use central difference formulas to approximate to the derivatives. The quantities v and p are discontinuous at the shock and hence two values a finite distance apart and equidistant from the shock front cannot approximate to the derivative. These difference formulas, less accurate than those in the body of the calculation,

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$$\frac{\partial v}{\partial r} = \frac{v_s - v_{i-\frac{1}{2}}}{r_s - r_{i-\frac{1}{2}}}, \quad \frac{\partial p}{\partial r} = \frac{p_s - p_{i-\frac{1}{2}}}{r_s - r_{i-\frac{1}{2}}} \quad (88)$$

are used. (i is here the mass point nearest the shock.)

The quantities to be obtained from the application of the shock conditions are the position of the shock and of the mass point, i, nearest to the shock. To calculate the position of point i, the difference equation (71) is used except that (88) is used to approximate $\frac{\partial p}{\partial r}$. Here as in the computation of $\frac{dv}{dt}$, a small error is made because of the failure to use a central difference formula.

The procedure used in computing the position of the shock is so complicated that it is impractical to use I.B.M. machines for it, but it can be done satisfactorily with an ordinary calculating machine. The steps in the calculation can be arranged on a computation sheet so that the time required to work out a cycle on it is of the same order of magnitude as the time for the machine cycle. If one person does the hand calculations and one person operates the machines, the time of a cycle need not be significantly increased.

With (87) expressing the acceleration of the shock, the position of the shock could be calculated from the second difference formula

$$r_s^{n+1} = 2r_s^n - r_s^{n-1} + \frac{\Delta t}{2} \left(\frac{d^2 r_s}{dt^2} \right)^n$$

However, in this form an error in r_s at one cycle affects the velocity as well as position in later cycles, and hence it may give rise to long period oscillations. The situation here is more serious than in the solution of Equation (71), for the shock pressure and velocity are more sensitive to the pressure difference than the corresponding quantities for a material point. Consequently the oscillations produced by an error may be of longer period and larger amplitude. A more stable formula is

$$r_s^{n+1} = r_s^n + \frac{1}{2} \left[\left(\frac{dr_s}{dt} \right)^n + \left(\frac{dr_s}{dt} \right)^{n-1} \right] + \frac{\Delta t^2}{2} \left(\frac{d^2 r_s}{dt^2} \right)^n$$

If this equation is used, an error in r_s does not produce a significant

error in the velocity of the shock and hence it is more quickly "corrected" by the pressure differences.

In the calculation of $\frac{d^2r_s}{dt^2}$ and $\frac{dr_s}{dt}$, v_s , and $\frac{dv_s}{dt}$ are needed. If v_s and the results of the machine calculation at that cycle are known, $\frac{dv_s}{dt}$ can be computed from Equation (85). To get v_s^n it is not accurate enough to use $\left(\frac{dv_s}{dt}\right)^{n-1}$ but $\left(\frac{dv_s}{dt}\right)^{n-\frac{1}{2}}$ is needed. To calculate $\left(\frac{dv_s}{dt}\right)^{n-\frac{1}{2}}$ directly $v_s^{n-\frac{1}{2}}$ would be needed. The best procedure is to use the formula

$$\left(\frac{dv_s}{dt}\right)^{n-\frac{1}{2}} = \frac{1}{2} \left(\frac{dv_s}{dt}\right)^n + \frac{1}{2} \left(\frac{dv_s}{dt}\right)^{n-1}$$

and an iteration method. v_s^n is guessed and $\left(\frac{dv_s}{dt}\right)^n$ is computed. Then a new v_s^n is calculated and this value used to compute a new $\left(\frac{dv_s}{dt}\right)^n$. This process is continued (it is rapidly convergent) until the same v_s^n is obtained from the formulas as was put into them.

A computation sheet can be set up which provides space for the computing of the various elements of the formulas and the combination of these elements into the desired quantities. Each item on the computation sheet should be in a form such that its computation requires only performing a single operation on a calculating machine or looking up the item in a table, with a possible linear interpolation. By a single operation on a calculating machine is meant a computation in which no intermediate writing down of a number is needed, e.g., $a(b + c)/d$.

The pressure table is often made up with the specific volume normalized so that the normal specific volume is 1, instead of v_0 . The following sample computation sheet was made up on the basis of this normalization. It is also assumed that the points are chosen equally spaced in r .

1. cycle: n

2. point nearest the chock: i

3. $r_s^n = r_s^{n-1} + \frac{\Delta t}{2} \sqrt{v_0} \left(W_1^{n-1} + W_1^{n+2} \right) \frac{(\Delta t)^2}{2} \sqrt{v_0} (Q^{n-1})$

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(This W^n differs from the one defined in (33) by a factor $\sqrt{v_0}$ Q^{n-1} differs from $\frac{d^2 r_s}{dt^2}$ by the factor $\sqrt{\frac{v_0}{2}}$.

4. $\Delta r_s^n = r_s^n - r_s^{n-1}$. This item is for checking purposes only. Jumps in the value of Δr_s^n indicates an error in r_s^n .
5. $\delta = r_s^n - r_i^{n-\frac{1}{2}}$. r_i^n is the value of r for the point which at cycle n is nearest the shock.
6. $\left(\frac{v}{a}\right)_{i-\frac{1}{2}}^n = y_{i-\frac{1}{2}}^n$ from I.B.M. listing.
7. $p_{i-\frac{1}{2}}^n$ from I.B.M. listing.
8. $v_{i-\frac{1}{2}}^n = \left(\frac{v}{a}\right)_{i-\frac{1}{2}}^n / \left(\frac{1}{a}\right)_{i-\frac{1}{2}}$. Items 1 - 8 are independent of the iteration procedure used in computing v_s^n .
9. v_s^n (guess).
10. ψ^n from table.
11. ω^n from table. $-\frac{\Delta \psi^n}{\Delta v} = \omega^n$
12. $A^n = 1 - v_s^n$
13. $(W^n)^2 = (\psi^n - p_0) / A^n$
14. $W^n = \sqrt{(W^n)^2}$. (This W^n differs from the one defined in (33) by a factor $\sqrt{v_0}$)
15. $G^n = \left[\frac{.75}{\sqrt{v_0}} (W^n)^2 + \frac{.25}{\sqrt{v_0}} \omega^n \right] / W^n$
16. $H^n = \frac{(\psi^n - p_0) (v_s^n / v_0)}{r_s^n}$
17. $M^n = \left[(W^n)^2 (1 - v_{i-\frac{1}{2}}^n / v_0)^{4.5} p_{i-\frac{1}{2}}^n + p_0 \right] / \delta$
18. $\left(\frac{dv_s}{dt}\right)^n = \left[H^n + .5 M^n \right] / G^n$
19. $v_s^n = v_s^{n-1} + \frac{\Delta t}{2} \left[\left(\frac{dv_s}{dt}\right)^n + \left(\frac{dv_s}{dt}\right)^{n-1} \right]$

If item 19 is not the same as item 9, a new v_s^n should be guessed and steps 9 - 19 repeated.

$$20. B^n = v_o (\psi^n - p_{i+\frac{1}{2}}^n) / \delta$$

$$21. R_i^{n+1} = 2R_i^n - R_i^{n-1} + (\Delta t)^2 B^n \text{ (Implosion)}$$

Card i is kept out of machine operations 1 and 2. Its R, computed in item 21, is hand punched into the appropriate columns and the card is released to the deck before operation 3.

$$22. U^n = A^n W^n \sqrt{v_o}$$

$$23. Q^n = - \left(\frac{dv_s}{dt} \right)^n \left[\omega^n - (W^n)^2 \right] v_o / U^n$$

Since the shock moves with respect to the material, it passes a new point every few cycles and then a new card must be added to the machine calculations. The time t^* , at which the shock wave hits the new point is determined by interpolation. In this interpolation W^{n+1} and consequently v_s^{n+1} are needed; hence these quantities at time $n + 1$ must be calculated. The shock specific volume at time t^* , v^* , is calculated by linear interpolation. ψ^* and u^* are obtained from v^* . The assumption is made that in the time from cycle n to t^* , the acceleration of a mass point at the shock front has not changed significantly, so B^n is used. The R at cycle $n + 1$ of the new point is gotten by expanding it in a power series in time about t^* . Since in a precise calculation of $v_s^{n+1}, v_{i+\frac{1}{2}}^{n+1}$ is needed, and to calculate $v_{i+\frac{1}{2}}^{n+1}$ the position of the new point is needed, an iteration method must be used. The first v_s^{n+1} used is the guessed v_s^{n+1} (item 9). When the new R is calculated, $v_{i+\frac{1}{2}}^{n+1}$ is calculated by hand and is used in getting a new v_s^{n+1} . The process is repeated until it has converged.

$$24. r_{i+1}^n \text{ from previously prepared table of the positions of the points.}$$

If r_s^{n+1} is less than r_{i+1}^n , items 25-49 need not be computed. If r_s^{n+1} is greater than r_{i+1}^n , the shock has hit point $i + 1$ between cycles n and $n + 1$, and items 25-49 must be computed.

$$25. t_{1,} = (r_{i+1}^n - r_s^n) / W_1^n. \text{ The first approximation to the time (multiplied by a } \dots \text{)}$$

factor $\sqrt{v_0}$ the shock hit point t_2 is another approximation to the time the shock hit point $i+1$.

26. $t_2 = (r_s^{n+1} - r_{i+1}^n) / W^{n+1}$; $\Delta t = t_2 - t_1$ is another approximation to the time the shock hit point $i+1$.

27. $t^* = t_1(2 \Delta t \sqrt{v_0} - t_1 - t_2) / (v_0 \Delta t)$, t^* is an average of t_1 and t_2 , with t_1 weighted by $\frac{\Delta t - t_1}{\Delta t}$ and t_2 by $\frac{t_1}{\Delta t}$. The factors v_0 and $\sqrt{v_0}$ are to remove the factor $\sqrt{v_0}$ in $t_1 + t_2$.

28. $\Delta t - t^*$

29. $(\Delta t - t^*)^2 / 2$

30. $(t^*)^2 / 2$

31. $v^* = [v_s^n (\Delta t - t^*) + v_s^{n+1} t^*] / \Delta t$

32. ψ^* from table.

33. $(U^*)^2 = \psi^*(1 - v^*) / (\frac{1}{v_0})$

34. $U^* = \sqrt{(U^*)^2}$, the velocity of point $i+1$ just after it was hit by the shock.

35. $R_{i+1}^{n+1} = r_{i+1}^n + U^* (\Delta t - t^*) + \frac{1}{2} (\Delta t - t^*)^2 B^n$

36. $R_{i+1}^n = r_{i+1}^n - U^* t^* + \frac{1}{2} (\Delta t - t^*)^2 B_n$

37. $(\frac{1}{a})_{i+1}$ from table

38. $(\frac{1}{a})_{i+\frac{1}{2}} = .375 (\frac{1}{a})_{i+1} + .750 (\frac{1}{a})_i - .125 (\frac{1}{a})_{i-1}$
quadratic interpolation.

39. $(\frac{1}{a \Delta r^3})_{i+\frac{1}{2}} = (\frac{1}{a})_{i+\frac{1}{2}} (\frac{1}{\Delta r^3})_{i+\frac{1}{2}}$. This is punched on card $i + 1$.

40. $Y^* = v^* (\frac{1}{a})_{i+1}$

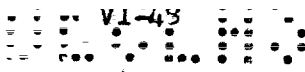
41. $F_1^* = F_1(Y^*)$ from table.

42. $F_2^* = F_2(Y^*)$ from table.

43. $b_{i+1} = (\psi^* - F_1^*) / F_2^*$

44. $b_{i+\frac{1}{2}} = .375 b_{i+1} + .750 b_i - .125 b_{i-1}$. This is punched on card $i + 1$.

45. $(R_{i+1}^{n+1})^3$



46. $(R_{i+1}^{n+1})^3$

47. $y_{i+\frac{1}{2}}^{n+1} = \frac{1}{(a \Delta r^3)_{i-\frac{1}{2}}} \left[(R_{i+1}^{n+1})^3 - (R_i^{n+1})^3 \right]$

This is the same as item 6 of cycle $n + 1$.

48. $R_{i+\frac{1}{2}}^{n+1} = F_1 (y_{i+\frac{1}{2}}^{n+1}) + b_{i+\frac{1}{2}} F_2 (y_{i+\frac{1}{2}}^{n+1})$

same as item 7 of cycle $n + 1$.

49. $v_{i+\frac{1}{2}}^{n+1} = y_{i+\frac{1}{2}}^{n+1} / \left(\frac{1}{a}\right)_{i-\frac{1}{2}}$

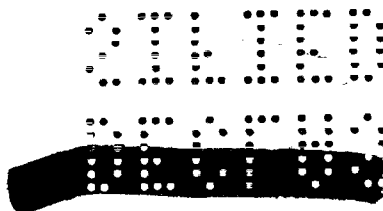
same as item 8 of cycle $n + 1$.

6.4-6 Card Layout.

If the number of intervals in r is chosen just large enough to give a good definition of the pressure curve, seven digits must be used in R . The number of digits in R determines the number of digits in other quantities: e.g., then v must have 5 digits. The columns of the card must be apportioned among the various quantities so that there is space for all of them and so that the columns allotted to those numbers punched by a multiplier are the same as the spacings given by available skip bars.

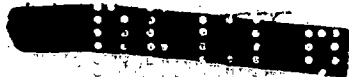
All the numbers to be punched on a card during a single cycle were found to occupy more than 80 columns. It was therefore necessary to use two cards to represent each point. This was accomplished without producing an increase in the time required for or the number of operations in a cycle. Each cycle uses two decks of cards. Deck 1 is used in operations 1-4. Since 4 is a reproducer operation, the necessary data can be transferred from deck 1 to deck 2 without any essential complication. Deck 2 is used from operation 4 on.

The distribution of card columns is given in the following table:



DECK 1

<u>Columns</u>	<u>Quantity</u>
1-2	Problem Number
3-5	Card Number
6-10	Time (cycle number)
11-16	$\frac{v_0}{a_{i-1/2}(\Delta r^3)_{i-1/2}}$
17-23	R_i^n
24	X-punch for sign of dP
25-31	$2R_i^{n-1} - R_i^{n-2}$
32	blank
33-40	$(R_i^n)^3$
41	X-punch to control shift in decimal of R^3
42-48	R_i^{n-1}
49	X-punch to control shift in decimal of R^3
50-56	(dP_i^{n-1})
57	blank
58	X-punch to control shift in decimal of R^3
59	blank
60-65	$\frac{v_0(\Delta t)^2(R_i^{n-1})^2}{r_i^2 \Delta r}$
66-72	$b_{i-1/2}$
73-78	$\frac{v_0(\Delta t)^2}{r_i^2 \Delta r}$
79-80	Δt



VP-50
DECK 2

"X" in 11 and 80 on all cards

<u>Columns</u>	<u>Quantity</u>
1-2	Problem number
3-5	Card number
6-10	Time (cycle number)
11-15	v_0
17-23	$a_{i-\frac{1}{2}} (\Delta r^3)_{i-\frac{1}{2}}$
24-30	F_1
31-35	blank
36	$v_{i-\frac{1}{2}}^n$
37-42	blank
43	last 6 digits of $(R_i^n)^3$
44-49	blank
50	last 6 digits of $(R_{i-1}^n)^3$
51-57	blank
58-65	$p_{i-\frac{1}{2}}^n$
66-72	blank
73-79	$b_{i-\frac{1}{2}}$
	F_2

For an explanation of the X-punches, see the subsection 6.4-7.

6.4-7 The Machine-Operations.

The elementary operations which make up a cycle are listed in 6.4-4. Here they are described in detail and plugboard wiring diagrams are given. Operation 1 - Triple product multiplier. R_i^{n-1} is squared on the first multiplication cycle and $(R_i^{n-1})^2$ is multiplied by $\frac{v_0 (\Delta t)^2}{r_i^2 \Delta r}$ on the second multiplication cycle. R_i^{n-1} is read from columns 42-48 into the multiplier and multiplicand counters, and $\frac{v_0 (\Delta t)^2}{r_i^2 \Delta r}$ is read from columns 73-78 into the summary counter. The product of the multiplication is punched into columns

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17-23. See Figure 8.

Operation 2 - Multiplier. Computation of R_1^{n-1} .

$2R_1^{n-1} - R_1^{n-2}$ is read from columns 25-31 into the summary counter.

$\frac{V_0 (\Delta t)^2}{r_1^2 \Delta r} (R_1^{n-1})^2$ is read from columns 60-65 into the multiplier counter,

and $|dP_1^{n-1}|$ is read from columns 50-56 into the multiplicand counter. The product is transferred from the products counter into the summary counter

positively if there is no X-punch in column 24 and negatively if there is an

X-punch in column 24. The result $R_1^n = (2R_1^{n-1} - R_1^{n-2}) + \frac{V_0 (\Delta t)^2}{r_1^2 \Delta r} (R_1^{n-1})^2 (dP_1^{n-1})$

is punched in columns 17-23. See Figure 9.

Operation 3 - Triple product multiplier. Computation of $(R_1^n)^3$. R_1^n is read from columns 17-23 into the multiplier, multiplicand, and summary counters.

On the first multiplication cycle, R_1^n is squared; on the second multiplication cycle, the cube is completed. The product, $(R_1^n)^3$ is punched in columns 33-40.


In many problems, R varies by a factor 10 in a single deck. Then R^3 in that deck varies by a factor 1000. Since this setup allows for the punching of only 8 digits of R^3 , the number of significant digits of R^3 punched could, for some cards, be as low as 5. This would result in a real loss of accuracy. However, by the use of two control X-punches, one in column 49 (see operation 4 for the role of X in 41.) and one in column 58, it is possible to have a sufficient number of digits of R^3 punched in all cards.

The X punch in 49 controls the digits of R^2 that are transferred from the products counter to the multiplier counter. 9 digits of R^2 are wired into a selector that is activated by the "X" in 49. The right hand 8 digits are wired into 8 "NX" hubs of the selector; the left hand 8 digits are wired into the corresponding 8 "X" hubs of the selector. Split wires are used for the 7 digits that are wired to both "X" and "NX" hubs of the selector. The 8 C hubs of these

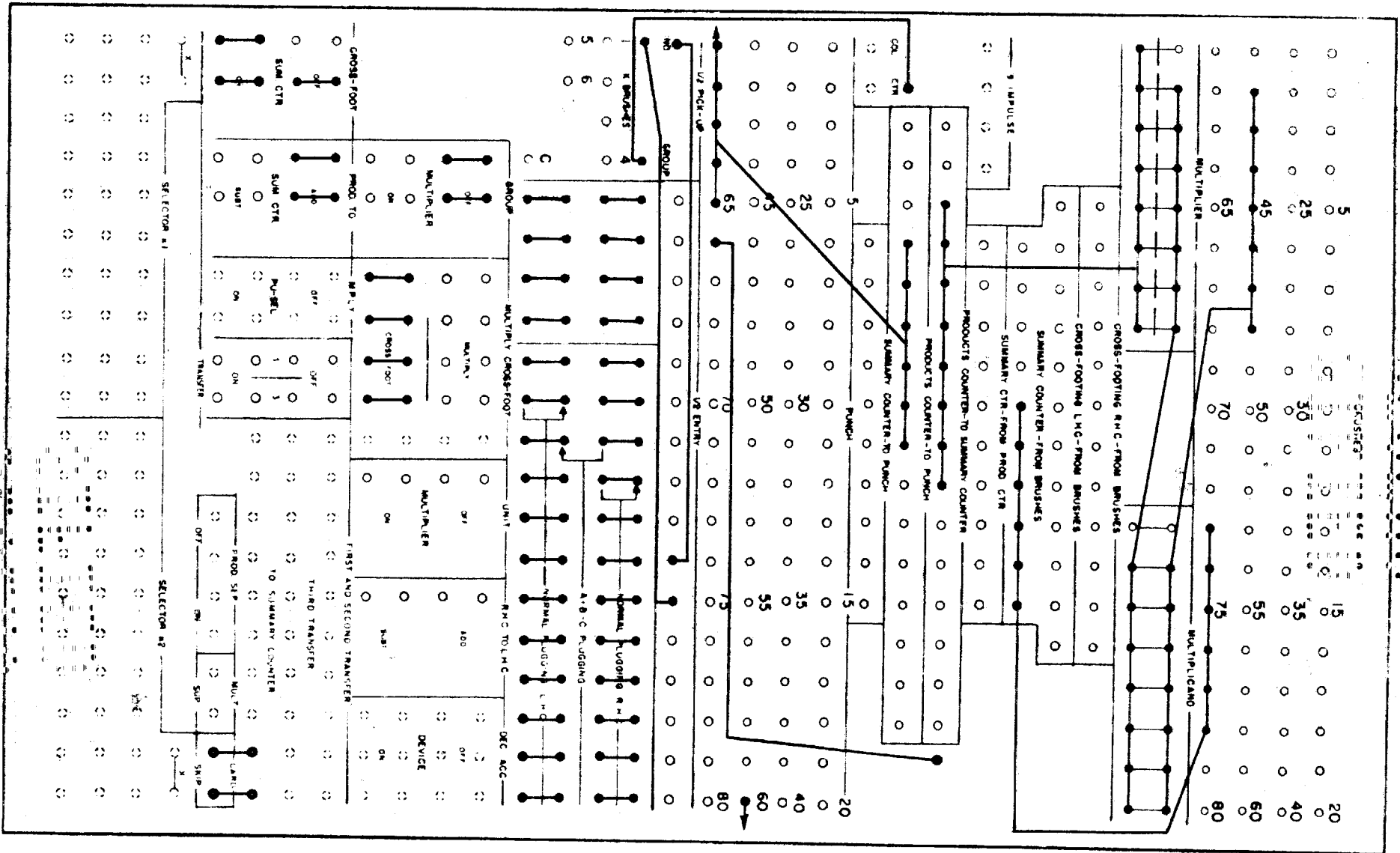
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Figure 8

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Figure 9

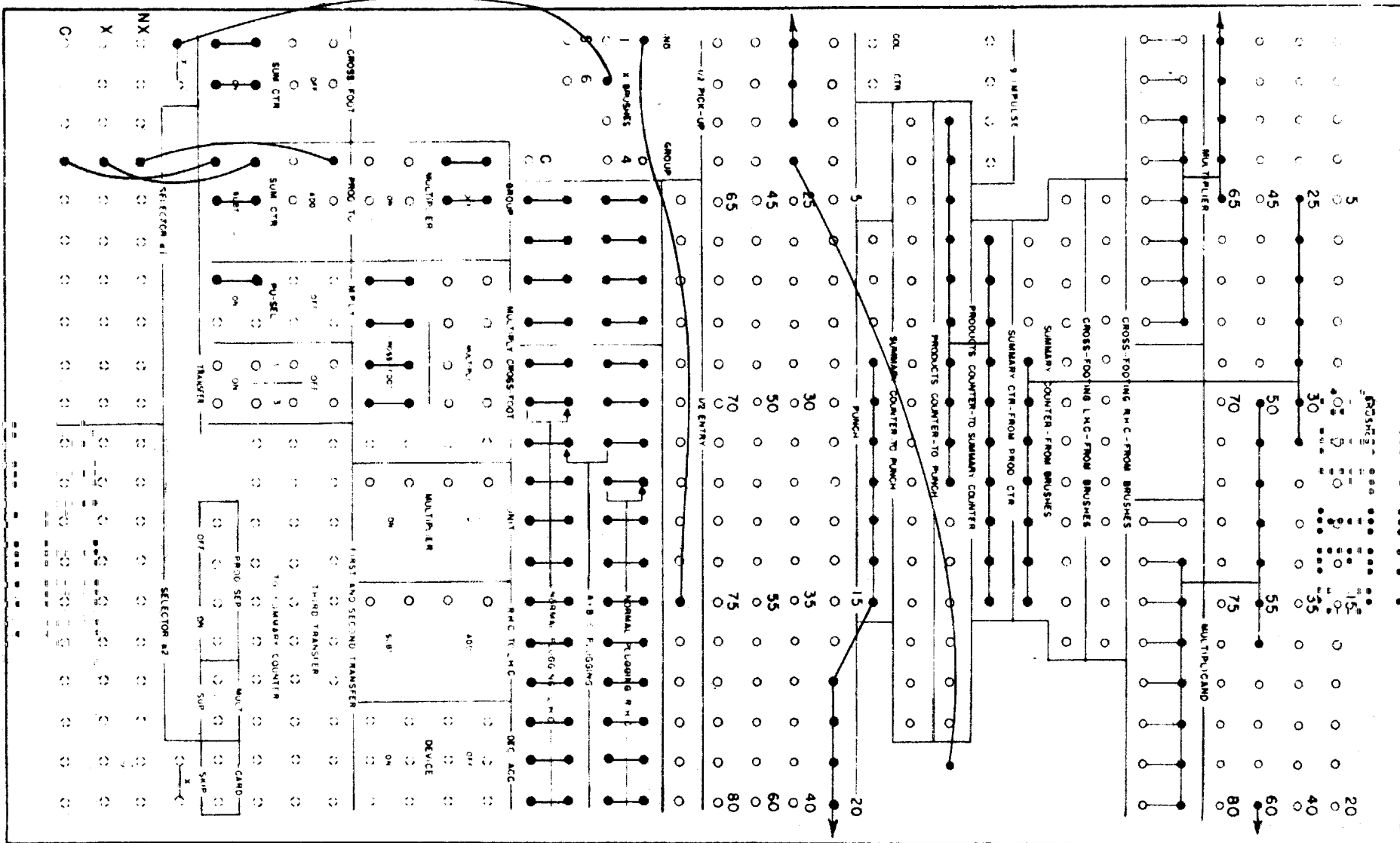
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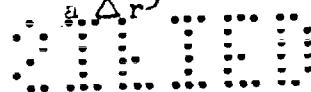


selector positions are wired into the multiplier counter. Thus the "X" in 49 shifts the decimal point in R^2 , as it appears in the multiplier counter, one position to the right; consequently, it shifts the decimal point in R^3 , as it is punched in the card, one column to the right.

The X-punch in column 58 controls the digits of R^3 that are punched. 10 digits of R^3 are wired from the products counter into the selector that is activated by the "X" in 58. The right hand 8 of these are wired into 8 "NX" hubs of the selector; the left hand 2 are wired into the "X" hubs of these 8 selector positions. Again split wires are used for the 6 digits that are wired into both "X" and "NX" hubs. The 8 C hubs of these selector positions are wired to the punch. Thus the "X" in 58 shifts the decimal point in R^3 , as it is punched in the card, two positions to the right. X-punches in both 49 and 58 shift R^3 three columns to the right. The plugboard wiring diagram is given in Figure 10.

Operation 4 - Reproducer. In this operation data necessary for the remaining operations are transferred from deck 1 to deck 2. In addition, R^3 of card 1-1 is transferred to card 1. This transfer makes possible the calculation of v in operation 5 from data on a single card. Since v is computed to only 5 digits, the difference of R_1^3 and R_{1-1}^3 need not have more digits. For convenience, however, the difference is allowed to run to 6 digits; that is, it is given the range 010000 to 999999. Since the difference of R^3 never has more than 6 digits, only 6 digits of R^3 need be used in performing the operation. Therefore, only the last 6 digits of R^3 are transferred from deck 1 to deck 2.

The following quantities are transferred directly from deck 1 into the same columns in deck 2. The problem number, col. 1-2; card number, col. 3-5; cycle number, col. 6-10; the rate $\frac{v_0}{a \Delta r^3}$, col. 10-16; and the rate b ,

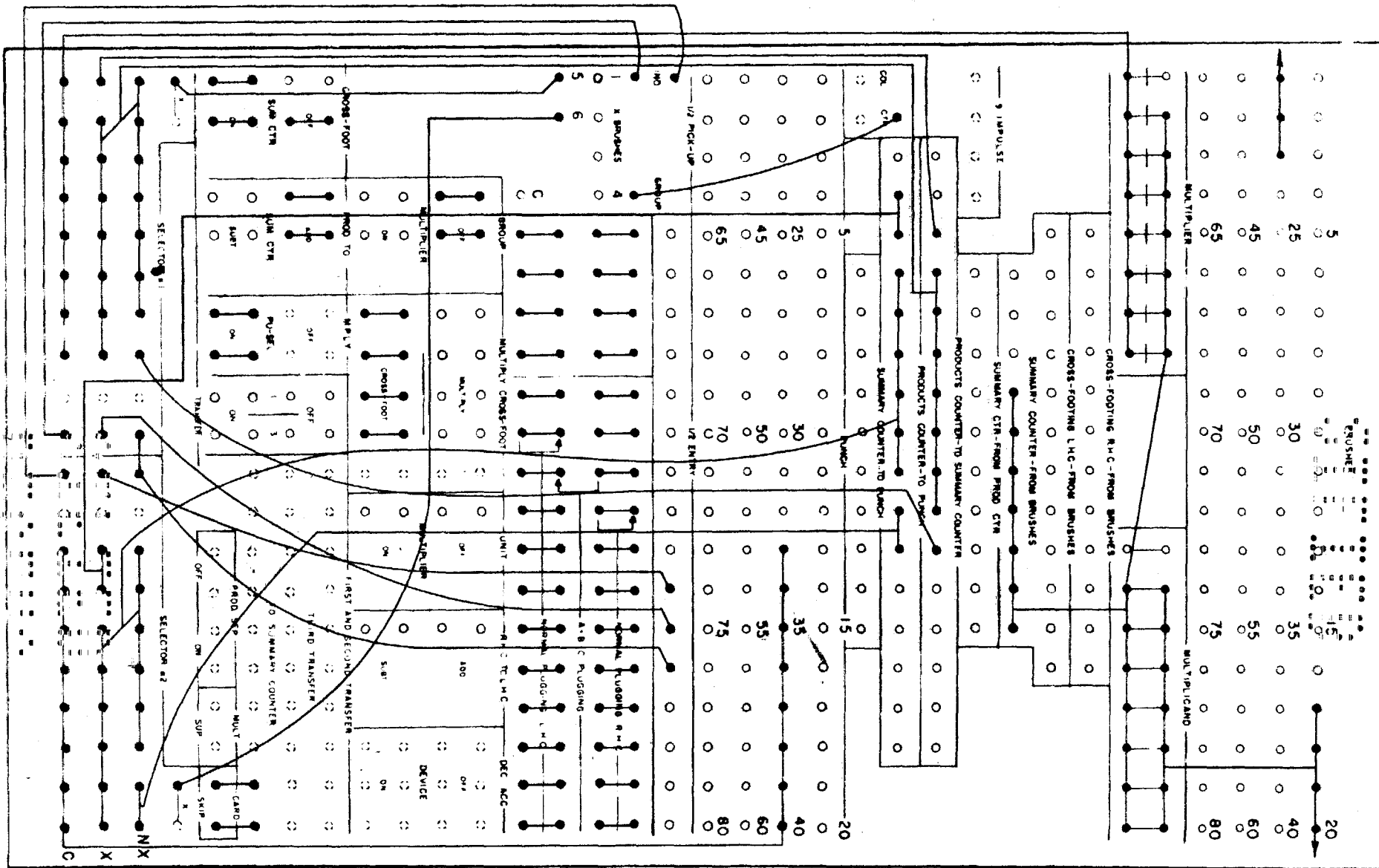


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Figure 10

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col. 66-72. An "X" from the 0 and X emitters is wired through the column split and punched in columns 11 and 60 on all cards of deck 2.

The last 6 digits of $(R_1^n)^3$ are transferred from columns 35-40 of deck 1 into columns 37-42 of deck 2; the last 6 digits of this quantity are transferred from columns 37-42 of card $i-1$ of deck 1 into columns 44-49 of card i of deck 2. In order for this operation to be performed, card $i-1$ must precede card i through the reproducer. On the other hand, in the tabulator-summary punch operation, operation 13, card $i+1$ must precede card i through the tabulator. Thus in operations 4 and 13 the cards must have a different ordering. In order to avoid a sorting operation, the cards are in both operations arranged in the order, card $i+1$ precedes card i , but in operation 4 the cards are run through the reproducer with the deck inverted so that the cards are face up, 12 edge first. This means that the hubs wired on the plugboard must be 81 minus the card column: e.g., card column 12 becomes plugboard $81 - 12 = 69$.

The existence of several decimal groups in R^3 , labeled by X-punches in columns 49 and 58, creates a problem in the transfer of R_{i-1}^3 , for the differencing of R^3 's in operation 5 is carried out in such a way that the 6 columns of R_i^3 and the 6 columns of R_{i-1}^3 should have the same decimal point position. Therefore, when card i belongs to one decimal group and card $i-1$ to another, a different type of transfer must be made than when both cards i and $i-1$ belong to the same decimal group. This is accomplished by transferring on that control situation the next to the last 6 digits of R^3 of card $i-1$ to card i . The X-punch, in 49, can be used to activate the selectors, three of which are needed. Since the reproducer sometimes fails to pick up a single X-punch, an "X" is punched in column 41, on all cards having an "X" in 49. It is unlikely that the reproducer would fail to pick up both X-punches on the same card.

As shown in the plugboard diagram, Figure 11, selector 1 and 3 are



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Figure 11

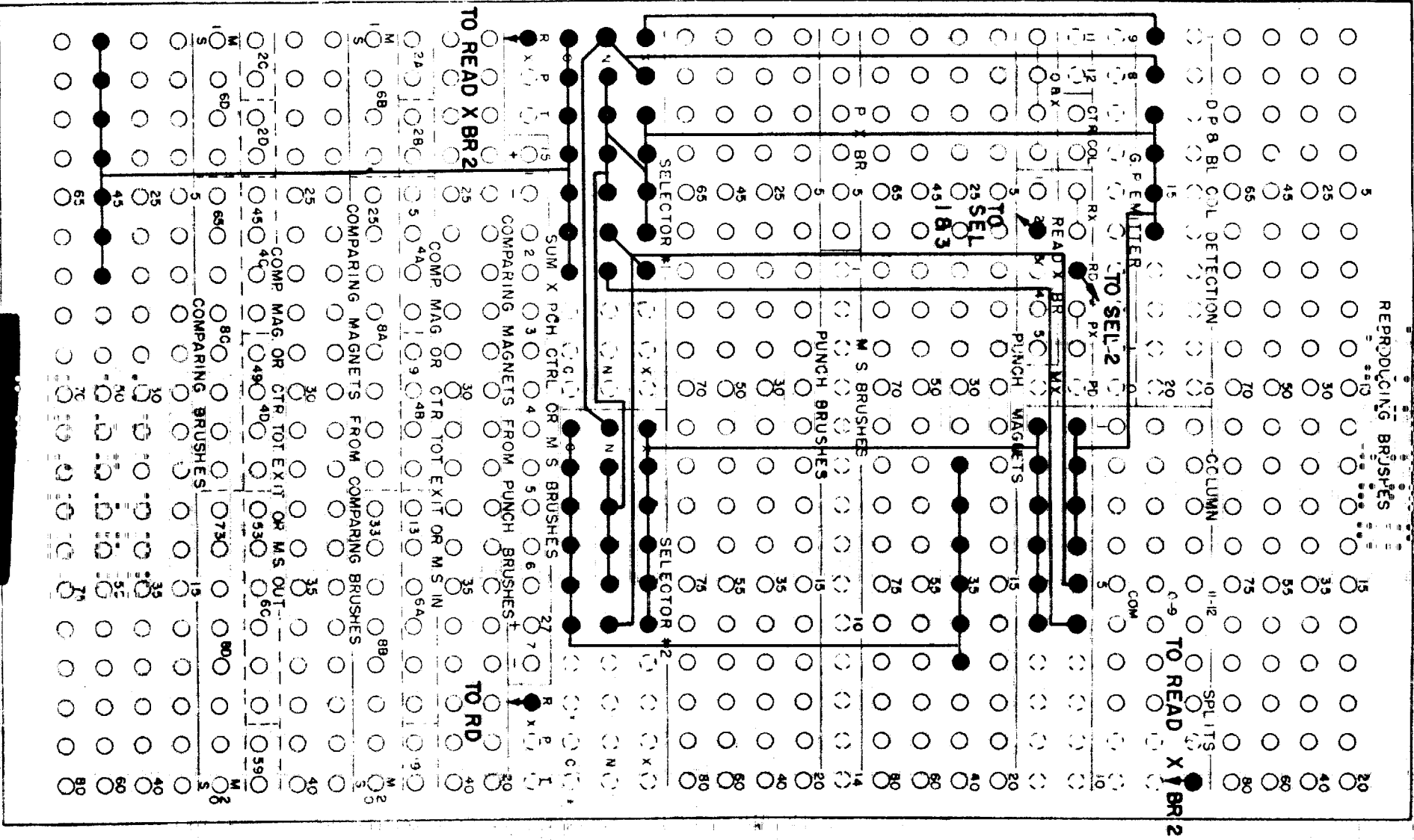
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INTERNATIONAL BUSINESS MACHINES CORPORATION
TYPE 513 AUTOMATIC REPRODUCING PUNCH PLUGBOARD
FOR SUMMARY PUNCHING - ALPHABETIC ACCOUNTING MACHINE

FORM 35 (1963 EDITION)
1700 PUNCH - EX-100

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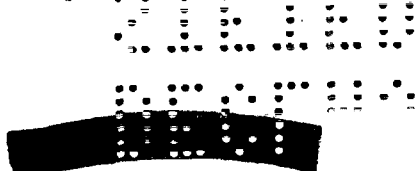
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activated directly by an X-punch in 41 and 49; selector 2 is also activated by the same X-punch, but through the cycle delay unit. Thus if neither card i-1 or i have an X-punch, all three selectors will be unselected; if both cards i and i-1 have X-punches, all three selectors will be selected. The selectors are wired so that in both of these control situations columns 35-40 of card i-1 of deck 1 are transferred into columns 44-49 of card i of deck 2. If card i has X-punches but card i-1 none, selectors 1 and 3 will be selected and selector 2 unselected; if card i has no punches but card i-1 does, selectors 1 and 3 will be unselected and selector 2 selected. They are wired so that in these two control situations columns 34-39 of card i-1 of deck 1 are transferred into columns 44-49 of card i of deck 2. For details, see Figure 11. Only the wiring of the selectors is shown in this figure. The wiring for the rest of the transfers is straightforward and is not shown. All subsequent operations use deck 2.

Operation 5 - Triple product multiplier. Computation of $(R_i^n)^3$ is read from columns 37-42 into the left hand components counter; $(R_{i-1}^n)^3$ is read from columns 44-49 into the right hand components counter, and the rate $\frac{v_0}{a_{i-\frac{1}{2}}(\Delta r^3)_{i-\frac{1}{2}}}$ is read into the summary counter. On the first multiplication cycle, the contents of the right hand components counter are transferred negatively into the left hand components counter, thus differencing R_i^3 and R_{i-1}^3 . On the second multiplication cycle, the difference of the R^3 's is multiplied by the rate. The product

$$\left(\frac{v}{a}\right)_{i-\frac{1}{2}}^n = \frac{v_0}{a_{i-\frac{1}{2}}(\Delta r^3)_{i-\frac{1}{2}}} \left[(R_i^n)^3 - (R_{i-1}^n)^3 \right] \text{ is punched in columns 31-35.}$$

Since on the first multiplication cycle, the right to left hand components counter transfer must be negative and on the second multiplication cycle, positive (in order for the multiplication to be done correctly), a special control must be provided. This control is accomplished through the use of the 2 position selector of the X-skip device. This selector, when activated, is selected only during the first multiplication cycle. An "X" control impulse is gotten from



the "X" in 80 punches on every card. See Figure 12.

The fact that R^3 in different decimal groups has its decimal point in different positions is taken care of by making a corresponding shift in the

$$\text{rate } \frac{v_0}{a_{i-\frac{1}{2}}(\Delta r^3)_{i-\frac{1}{2}}}.$$

Operation 6 - Sorter. Deck 2 is sorted into ascending order on the first three digits of v , columns 31-33. This sorting makes deck 2 ready for merging by the collator with the cards of the table of F_1 and F_2 .

Operation 7 - Collator. The work cards, deck 2, are merged with the table cards, which have been previously sorted into ascending order on their argument, a three digit v . The merging is such that the table card precedes the work card; hence the table cards are put in the primary feed hopper and the work cards are put in the secondary feed hopper. Those table cards that do not have a v that matches the v of any work card are selected out and put in stacker 1. The table cards are checked for sequence. Since they are supposed to be in ascending order, the low second primary hub is connected to the error stop hub. See Figure 13.

After the merged table cards have been used, they must be reinserted in their proper place in the table so that they can be used in the next cycle. This can be accomplished with the same plugboard as was used to merge the work and table cards if the instructions to select the primary and secondary cards are wired through a selector. The secondary X-selector is used and is activated by the "X" in 80 on the work cards. The table cards should not have an X-punch in column 80. See Figure 13.

Operation 8 - Multiplier. Interpolation of F_1 . F_1 is read from the table cards, interpolated and the result punched on the work cards. This can be done in one run of the cards through the multiplier if the table entries of F_1 have no more than 5 digits and the first differences of F_1 have no more than 3 digits. This limitation exists because F_1 and its first difference ΔF_1 are stored in the 8 position multiplier counter as a group multiplier

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00100

Figure 12

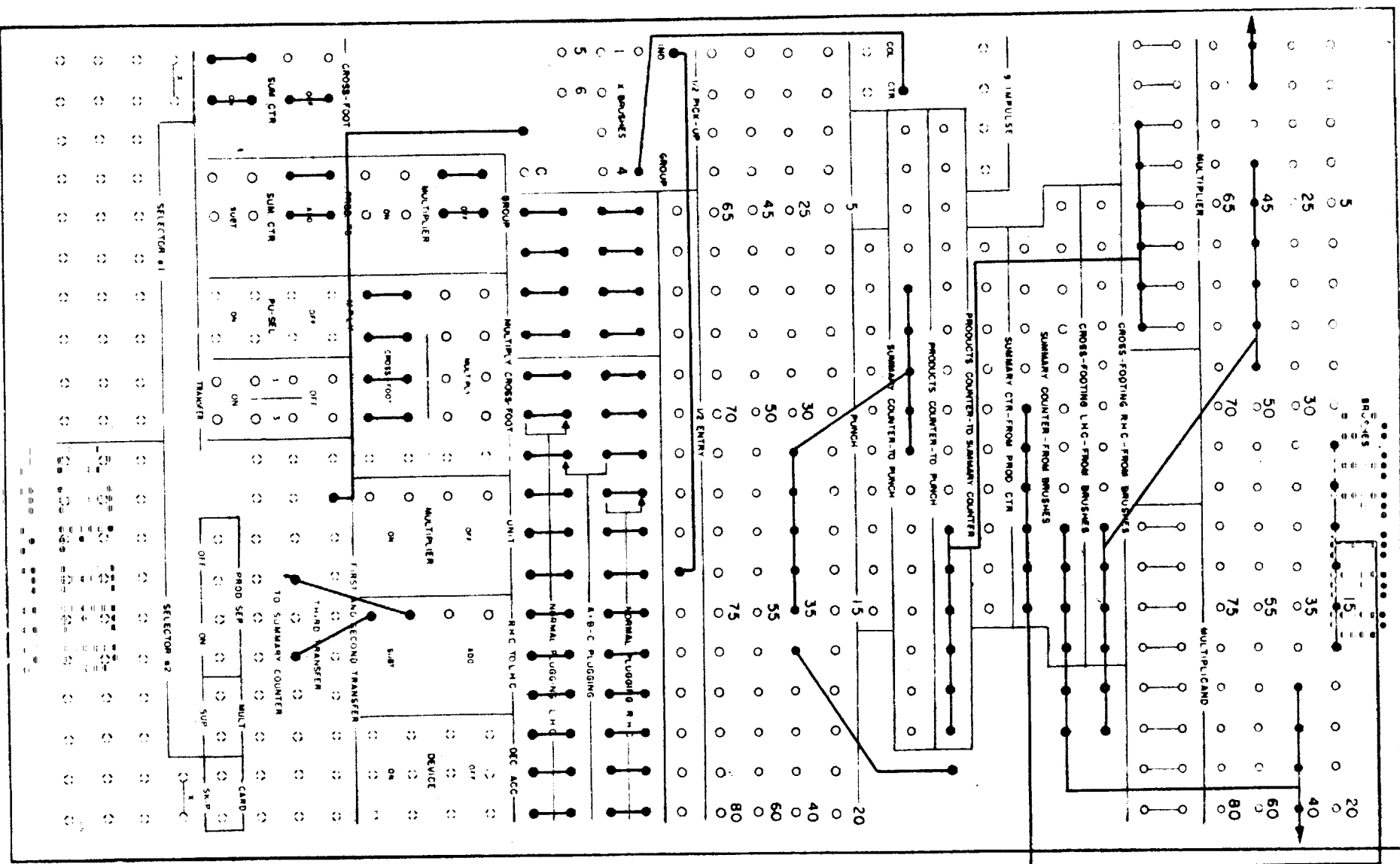
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ELECTROTYPE NUMBERS OF CARDS INVOLVED:

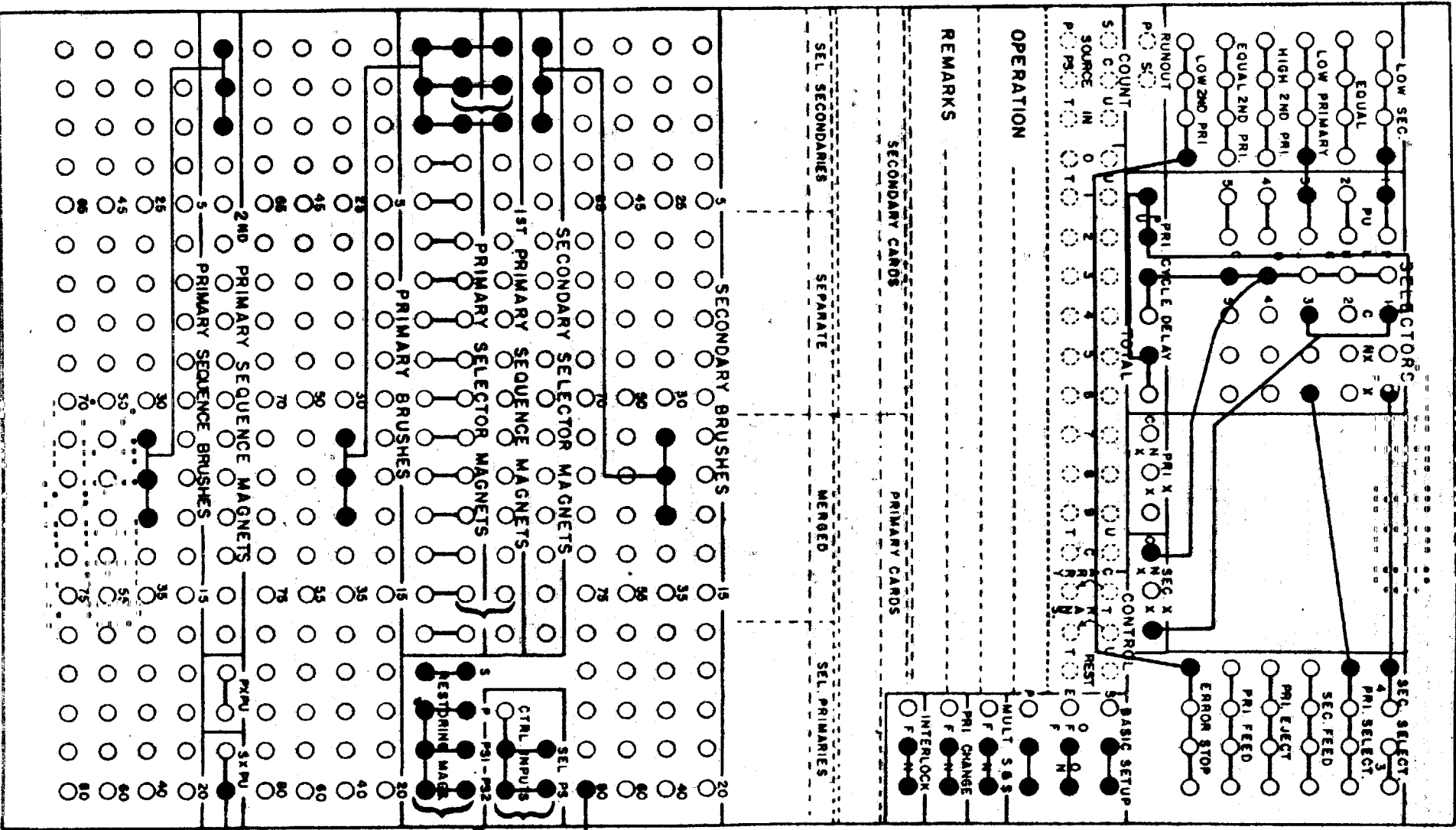
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Figure 13

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INTERNATIONAL BUSINESS MACHINES CORPORATION
TYPE 077 INTERNATIONAL COLLATOR PLUGBOARD



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DATE _____

DEPARTMENT OF CUSTOMER _____

to be used by the work cards. During the work card cycle, a unit impulse is entered in the extreme right hand position of the multiplicand counter and the last two digits of v , Δv are read from columns 34 and 35 of the work card into the two extreme left hand positions of the multiplicand counter.

The calculation to be performed is $F_1 + \Delta F_1 \Delta v$. F_1 is read into the right hand 5 positions of the multiplier counter and ΔF_1 into the remaining 3 positions. In the following multiplication the first three digits of the product $\Delta F_1 \Delta v$ are computed correctly. The fourth digit of that product has added to it the first digit of the product $F_1 \Delta v$; hence it is not correct. However, only three digits of $\Delta F_1 \Delta v$ are needed; the error in the fourth digit only affects the rounding. On this account the last digit of the interpolated value of F_1 will sometimes be wrong. The product $\Delta F_1 \Delta v$ must still be added to F_1 in order to complete the interpolation. To do this F_1 is wired from the multiplication table (it has been multiplied by 1) into the summary counter and $\Delta F_1 \Delta v$ is transferred from the products counter to the summary counter. This transfer is shown as negative in Figure 14 since in most equations of state ΔF_1 is negative. The fourth multiply-crossfoot switch is set on crossfoot in order to delay punching until the products to summary counter transfer has taken place. The upper hub of the second crossfoot switch is wired to the upper hub of the on setting of the second crossfoot to summary counter switch in order to permit the summary counter to receive the impulses from the multiplication table. See Figure 14.

During the course of a problem, p may vary by several factors of 10. Seven card columns in deck 2 have been allotted to p , F_1 and F_2 in order to allow for this variation. Of these seven digits of p that are punched, only 5 can be significant since the table entries from which p is computed have only 5 digits. However, this does not produce any error, since when p is large, small time intervals must be used (see §.4-3) and only the first 5 digits of it contribute to the value of R . When p is small, larger time intervals are used, but the significant 5 digits of p are then the right hand

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Figure 14

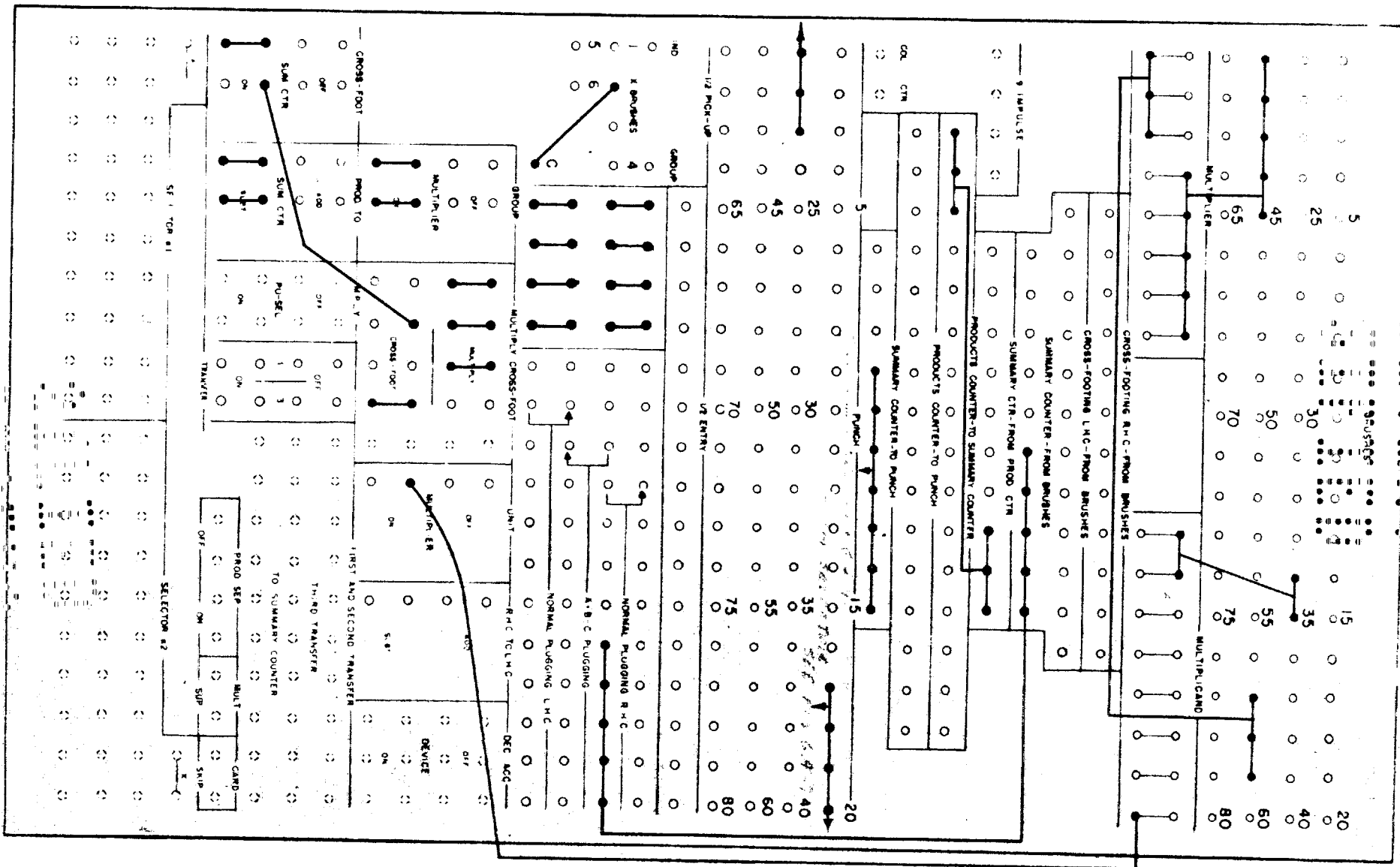
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INTERNATIONAL BUSINESS MACHINES CORPORATION

TYPE 601 MULTIPLIER

6-4042

FORM 32 9080-5 FNO
PAGE 45



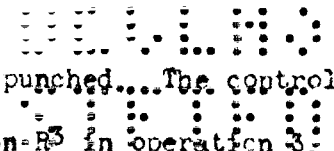
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TITLE OF REPORT _____

DATE _____

ELECTROTYPE NUMBERS OF CARDS INVOLVED: _____



 5 of the seven that are punched. The control on this variation in P is similar to the control on F_1 in operation 3. The pressure table is divided into several decimal groups, identified by X-punches in columns 73 and 76. These X-punches designate into which 5 card columns the interpolated F_1 is punched. They are read from the table card and the selectors they activate must remain selected until the last work card matched with that table card has been punched. The wiring of such an X-control is shown in Figure 15, where the X-punches in columns 80 and 11 of the work cards are used to keep the selectors activated. Figure 16 shows the wiring of the selectors to accomplish this control on the digits of F_1 punched. We have not found it necessary to use the full capacity of this system, so only 7 digits are shown wired to the punch. Although in an actual problem the features in Figure 14, Figure 15, Figure 16 are incorporated in one plugboard, they have been separated here to make the wiring more easily understood.

Operation 9 - Multiplier. The interpolation of F_2 is the same as for F_1 except that different card columns are used. In some problems bF_2 is small compared to F_1 . Then it is usually not necessary to interpolate F_2 , and $p = F_1 + bF_2$ can be computed without the intermediate punching of F_2 . F_2 is read as a group multiplier from the table card. From the work card, b is read into the multiplicand counter and F_1 is crossfooted into the left hand components counter.

Operation 10 - Sorter. The table cards are sorted out from the work cards. Column 1 can be used. Then all the table cards will fall in the reject pocket and all the work cards will fall in the pocket corresponding to the problem number.

Operation 11 - Multiplier. Computation of $P_{i-1/2}^n \cdot b$ is read into the multiplier counter, F_2 into the multiplicand counter, and F_1 into the left hand components counter. The result, $F_1 + bF_2$, is punched in columns 50-56. Since this is a standard type I.B.M. multiplier operation, no diagram is given.

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Figure 15

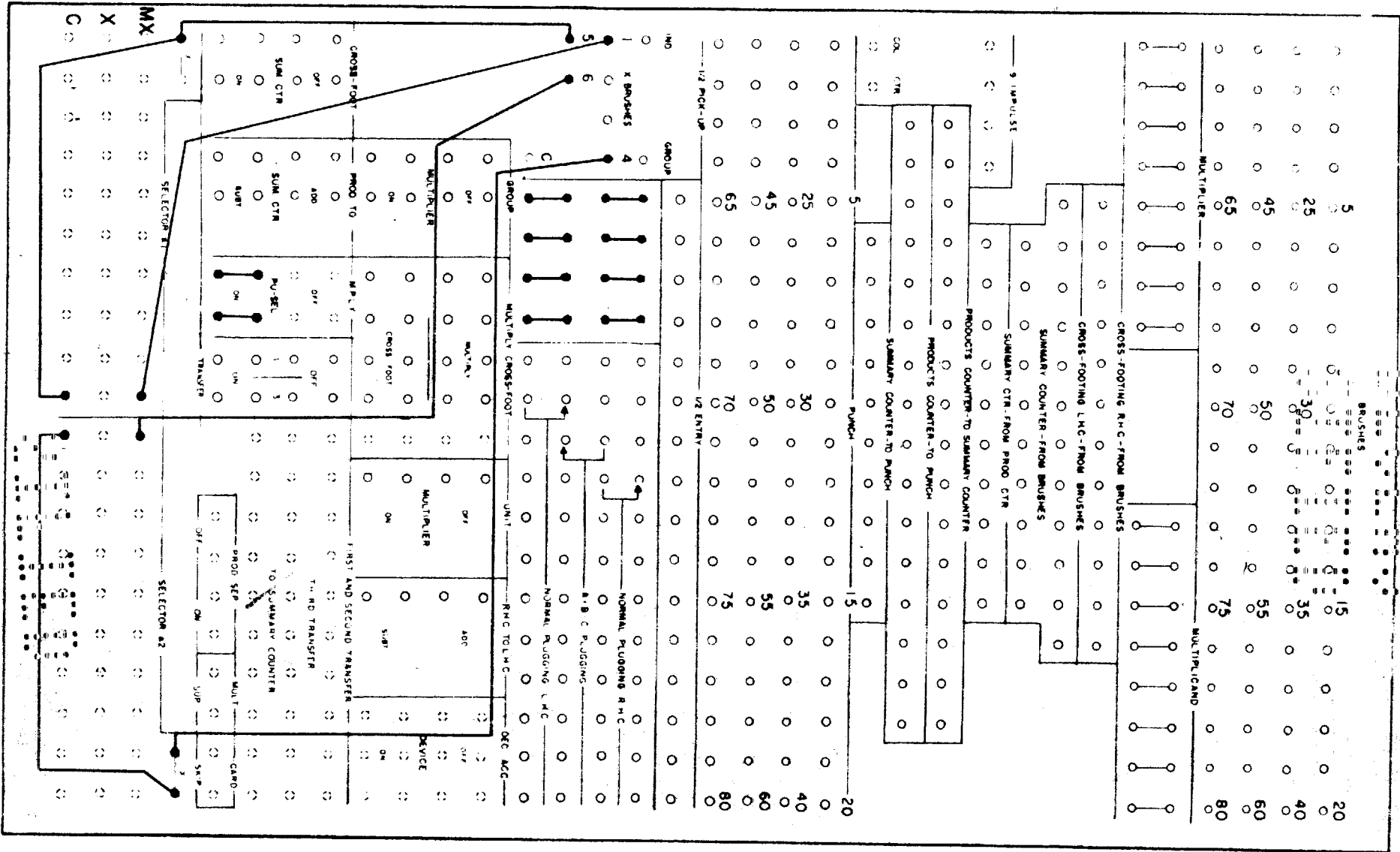
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TYPE 501 MULTIPLIER

6-4042

FORM 32 9080-5 END
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TITLE OF REPORT _____

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ELECTROTYPE NUMBERS OF CARDS INVOLVED:

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Figure 16

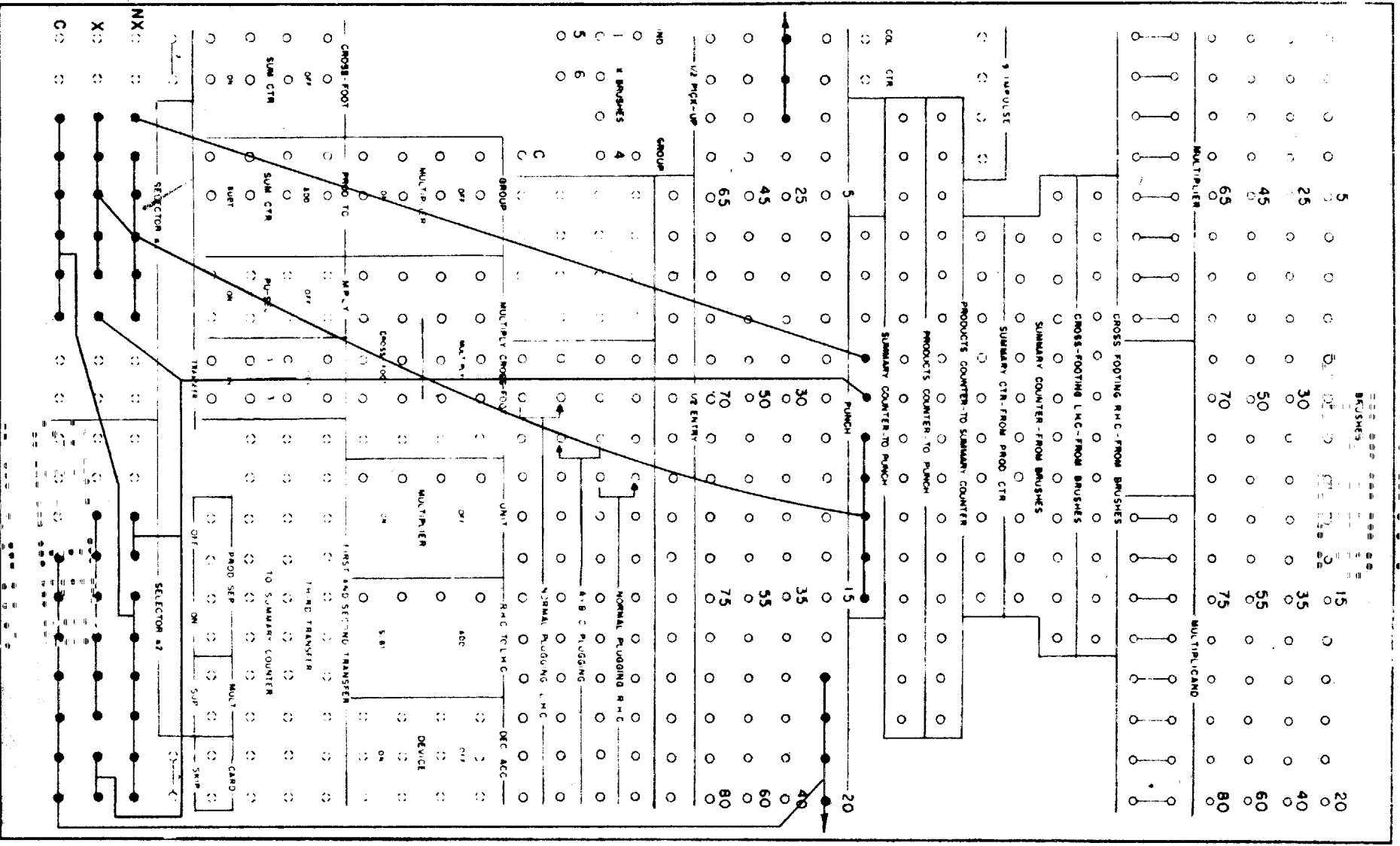
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TYPE 601 MULTIPLIER

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ELECTROTYPE NUMBERS OF CARDS INVOLVED:

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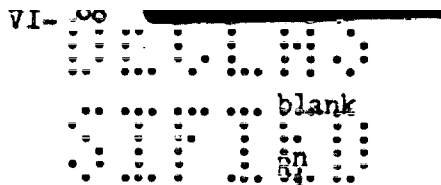
Operation 12 - Sorter. In the listing and differencing operations done by the tabulator-summary punch, numbers from both deck 1 and deck 2 are needed. Also 2 card cycles are needed to perform some of the computations. So deck 1 is merged with deck 2, the deck 1 card ahead of the corresponding deck 2 card. This is done by placing deck 1 in the feed hopper of the sorter and deck 2 on top of it. The cards are sorted into descending order on the card number, columns 3-5.

Operation 13 - Tabulator-summary punch. Information from decks 1 and 2 is listed. $R_i^n - R_i^{n-1}$ and dp_i^n are computed and listed. $2R_i^n - R_i^{n-1}$ and dp_i^n are computed and punched on deck 1 of cycle $n + 1$ in the summary punch. Identification, rates, and R_i^n are punched on the new deck.

The tabulator does not have enough type bars to print all the numbers punched on the cards and computed in this operation. The following choice of items gives the necessary information about the solution and includes useful checks on the calculation.

Alphamerical Type Bars

<u>Type Bars</u>	<u>Item Printed</u>
1-2	Problem Number
3-5	Card Number
6-10	Time (cycle number)
11	blank
12-13	time interval, Δt
14-20	$b_{i-\frac{1}{2}}$
21	blank
22	$\frac{v_o(\Delta t)^2}{r_i^2 \Delta r}$
29	blank
30-35	$\frac{v_o(\Delta t)^2}{r_i^2 \Delta r}$ $(R_i^{n-1})^2$



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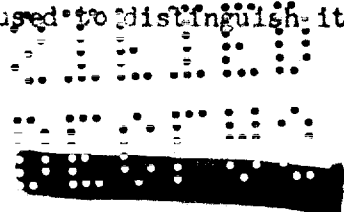
37-43

Numerical Type Bars

Type Bar	Item Printed
1-5	$R_1^n - R_1^{n-1}$
6	sign of $R_1^n - R_1^{n-1}$ (Cr symbol if negative, blank otherwise)
7-12	$\frac{v_0}{a_{i-1/2}(\Delta r^3)_{i-1/2}}$
13	X in 49 (asterisk)
14	X in 58 (Cr symbol)
15-22	R^3
23	blank
24-28	$v_{i-1/2}^n$
29	blank
30-36	$p_{i-1/2}^n$
37	blank
38-44	dp_1^n
45	Sign of dp_1^n (asterisk if negative, blank otherwise)

It was not always possible to have a blank space between each item printed. The items for which this omission occurs were chosen so that the least confusion resulted; e.g., the problem number and time are the same for all cards and hence do not interfere very much with reading the card number. Sometimes alphabetical characters are used for the problem identification, and in the early stages of the problem the time does not contain 5 digits. Only rarely does $b_{i-1/2}$ have 7 digits.

Since decks 1 and 2 are merged, there are two card cycles for each point i. The 'X' in 80 in deck 2 is used to distinguish it from deck 1. All three



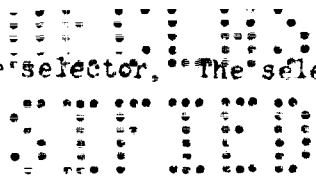
VI-69

list-tabulate switches are set to tabulate and a minor cycle is taken every two card cycles; hence, information concerning point i is printed on one line - first from the list cycle following the previous total cycle and then, without the platen moving, from the total cycle. In the following discussion, the card cycles are referred to in the following manner: at cycle one, the card from deck 1 is at the upper brushes; at cycle two, the card from deck 1 is at the lower brushes. The total cycle for that point is taken after the card from deck 2 passes the lower brushes; this gives time for the computing of $2R_1^n - R_1^{n-1}$.

The trickiest feature of the wiring is that for the computing of $2R_1^n - R_1^{n-1}$. On cycle 1, R_1^{n-1} is read by the upper brushes and entered negatively into a counter. On cycle 2, R_1^n is read by the lower brushes and entered positively into the same counter and also into another counter. Thus at the end of cycle 2 one counter contains $R_1^n - R_1^{n-1}$ and the other contains R_1^n . On the next cycle (cycle 1 again) the first counter, on a card cycle total transfer, transfers $R_1^n - R_1^{n-1}$ positively into the second counter forming $2R_1^n - R_1^{n-1}$. Then a total cycle is taken, clearing the counters. This operation has, of course, taken three card cycles and the first counter should have been receiving the impulses from the next card at the time it was transferring $R_1^n - R_1^{n-1}$ into the second counter. This difficulty is avoided by using two counters which alternately compute $R_1^n - R_1^{n-1}$.

For this computation two basic cycles of selector operation are needed, one of period 2 and the other of period 4. The one of period 2 is obtained simply by wiring an impulse from lower brush 80 to the X-pickup of a selector. When deck 2 passes the lower brushes, an "X" impulse comes through and activates the selector; when deck 1 passes the lower brushes, no "X" impulse comes through. Therefore, the selector is selected on cycle 2 and is unselected at cycle 1. The period of 4 is obtained by connecting lower brush 80 to an "X" position of a selector, upper brush 80 to "NX" of that selector position, and the C of that

position to the "X" pickup of the selector. The selector then goes through the following cycle.



- Cycle 1 unselected - (80 LB is connected to "X" and cannot activate selector for cycle 2)
- Cycle 2 unselected - (80 UB is connected to NX and hence activates selector for next cycle)
- Cycle 1 selected - (80 LB is connected to "X" and now can activate selector for next cycle.)
- Cycle 2 selected - (80 UB is connected to NX and cannot now activate selector for next cycle)

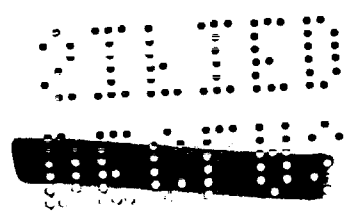
and repeat.

In Figure 17 selectors A and B operate on a period 2 cycle and selectors G, H, and C operate on a period 4 cycle.

Upper brushes 42-48 are wired to NX of a period 2 selector (selector A) and lower brushes 17-23 to the "X" of the same selector positions. The 7C hubs of these positions are connected to C of a period 4 selector. Thus the C of the period 4 selector receives on cycle 1, R_1^{n-1} , and on cycle 2, R_1^n . This period 4 selector (selector G) is used to enter R_1^{n-1} and R_1^n alternately into counters 8A and 8B. The X-hubs of selector G are wired to the 8A counter entry and the NX to the 8B counter entry.

- Counters 8A and 8B are used to compute $R_1^n - R_1^{n-1}$. Counter 8D is used to compute $2R_1^n - R_1^{n-1}$ and counter 8C is used to transfer R_1^n to the new deck in the summary punch.

Add-subtract impulses for the counter are timed in the following way: plug to C gives an impulse on both times 0 and 2; a plug to C impulse wired to a C hub of selector A gives rise to a time 1 impulse out of "NX" and a time 2 impulse out of X; a time 2 impulse wired to a C hub of selector G gives rise to time 2 impulses alternately coming out of "X" and "NX". The counters are impulsed as follows:



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Figure 17



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Counter	Time 1	Time 2
8A	+	on every other time
8B	-	on cycle 8A is not impulsed
8C	not impulsed	+
8D	+	+

Counters 8C and 8D are always clear on the total cycle. Counters 8A and 8B take turns clearing on the total cycle.

The counter total exits of counters 8A and 8B are wired into the "X" and "NX", respectively, of selector H. The C of selector H is wired to the C of selector B. The "NX" of selector B is wired to 8D counter entry. Thus 8A and 8B, alternately, on time 1, transfer $R_1^n - R_1^{n-1}$ into counter 8D, which on the preceding time 2 had R_1^n entered in it. If the totals from 8A and 8B were not wired through selector B but were connected directly to 8D counter entry, a back circuit would result when counters 4ABCD, which are used in computing dP , go through a conversion cycle. See Figure 17 for the wiring.

The tabulator is instructed to take a minor total cycle after cycle 1 by wiring lower brush 80 to digit selector 2. The 11 or "X" hub of digit selector 2 is wired to the comparing relays. On cycle 1, the "X" in deck 2 cards sends an impulse through this circuit. Since the comparing relays do not receive a matching impulse, an unequal impulse is generated. This is wired to the minor total hub.

The computation of $dP_1^n = P_{1-1/2}^n - P_{1+1/2}^n$ is similar to the computation of $R_1^n - R_1^{n-1}$. Two 8 position counters are used alternately. Since, 8A, 8B, 8C and 8D are already in use, two 8 position counters are made by connecting 4A to 4B and 4C to 4D. P is read into these counters from upper brushes 51-57 at time 2. The counters are impulsed alternately plus and minus at time 2. They receive no add or subtract impulse at time 1; hence no selectors are

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needed to control the counter entry impulses. Selector C, which operates on a period of 4, is used to control the impulses from the counter total exit to the type bars. If no selector is used here, a back circuit will result and wrong numbers will be printed. See Figure 17 for the plugboard wiring. The items that are listed and transferred are not shown in the wiring diagram. They are standard tabulator operations, and their presence in the diagram would require so many lines that the diagram would become almost unreadable.

X-punches are transferred from the decks of cycle n to deck 1 of cycle n + 1 by using them to direct a counter to go through a conversion cycle. Then the summary punch can be wired to punch an "X". The counter is made to go through a conversion cycle by wiring the add-subtract impulse through a selector activated by that "X". The selector is wired so that when it is controlled the counter subtract hub is impulsed. Then if the extreme left hand position of the counter has no digit entered in it and the CI and C hubs are wired to counter balance control, the counter will go through a conversion cycle.

The summary punch plugboard wiring diagram is also not shown. The totals of counters 4AB and 4CD must be wired to a selector and the common of the selector wired to the punch. If this is not done and a circuit connecting the punch to both counters at once is formed, wrong numbers will be punched.

6.5 THEORY OF VON NEUMANN'S METHOD OF TREATING SHOCKS (Peierls)

6.5-1 Introduction.

It is well known that in hydrodynamic problems involving compressible media there may exist shock waves, i.e., places at which the velocity, pressure and density are practically discontinuous, and at which the equations of Euler do not hold. The reason for this is that the Euler equations assume the changes in the material to be reversible, whereas at a shock wave gradients become so large that the dissipative effects (viscosity, heat con-

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VI 4

duction) become important. Indeed, in the limit usually considered, in which the dissipative terms are small in the units appropriate to the problem, the shock is a sharp discontinuity and the gradients are infinite.

Therefore, it would in general not make sense to assume Euler's equations to hold even across the shock. Von Neumann has pointed out, however, that the situation is different if one uses, instead of the differential equations, the approximate difference equations which are the basis of a mechanical method of treating the equations. In conditions where a shock would form, we know there exists no solution of the differential equations. Any solution of the difference equations will approximate to a solution of the differential equations only if the changes of all functions over one interval are small, hence the difference equations cannot be expected to have any solution of this kind at a shock. There are, however, solutions of oscillatory behavior containing fluctuations with periods of the order of the interval size. These, according to von Neumann, can be regarded as a model of the increase of entropy in the shock, and indeed the fluctuations thus obtained represent the heat motion of the shocked material.

It is evident that this model of the heat motion is very crude, and that it does not represent correctly the thermal behavior of any reasonable substance. However, there are many cases of interest in which the influence of temperature on the equation of state is negligible, and in those cases one may expect that the error introduced by the model may not be serious.

The purpose of this section is to study the difference between the model and an actual substance in more quantitative detail, and to derive criteria that may serve to estimate the error in individual cases.

6.5-2 Basic Equations.

In one case of a one-dimensional problem the differential equations are

$$\frac{\partial^2 y}{\partial t^2} = -\frac{1}{\rho_0} \frac{\partial p}{\partial x}$$

$$p = p(V), \quad V = \frac{\partial y}{\partial x}$$

(89)

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where y is the position at time t , of the point which would be at x if the material had normal density. p is pressure, which is assumed to be a unique function of the specific volume V (reversibility). More precisely V stands for the ratio of the volume to the normal volume. The normal density is ρ_0 .

The difference equation is obtained from this by choosing time intervals Δt and space intervals Δx , so that after neglecting higher than second powers of the interval sizes, (89) becomes:

$$\left. \begin{aligned} \frac{y_1^{n+1} - 2y_1^n + y_1^{n-1}}{(\Delta t)^2} &= - \frac{1}{\rho_0 (\Delta x)^2} (p_{i+\frac{1}{2}}^n - p_{i-\frac{1}{2}}^n) \\ v_1^n &= \frac{1}{\Delta x} (y_{i+\frac{1}{2}}^n - y_{i-\frac{1}{2}}^n) \end{aligned} \right\} \quad (90)$$

Where n, i , label the time and space intervals:

$$\begin{aligned} t_n &= n \Delta t + \text{const.} \\ x_i &= i \Delta x + \text{const.} \end{aligned} \quad (91)$$

We apply these equations to the state of affairs we expect behind a shock, where there will be irregular fluctuations superimposed on a "macroscopic" or mean motion. If our interval sizes are chosen correctly, the mean quantities vary little over one interval and over a few intervals we may regard all macroscopic quantities as uniform.

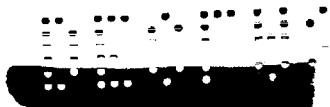
As to the "atomic" motion, or fluctuations, we shall assume that the amplitude is small. The limitations introduced by this assumption will be discussed later. We can then write

$$y_i^n = \bar{y}_i^n + \gamma_i^n \quad (92)$$

where the bar denotes the "mean" position and γ_i^n is small. Then

$$p_i^n = p(\bar{V}) + \left(\frac{dp}{dV} \right) \frac{1}{\Delta x} \left(\gamma_{i+\frac{1}{2}}^n - \gamma_{i-\frac{1}{2}}^n \right) \quad (93)$$

and (90) becomes:



$$\frac{\gamma_i^{n+1} - 2\gamma_i^n + \gamma_i^{n-1}}{(\Delta t)^2} = -\frac{1}{\rho_0(\Delta x)^2} \left(\frac{dp}{dv} \right) \bar{v} (\gamma_{i+1}^n - 2\gamma_i^n + \gamma_{i-1}^n) \quad (94)$$

Solutions of this equation can be written in the form

$$\gamma_i^n = A e^{j(n\phi + i\psi)} \quad j = \sqrt{-1} \quad (95)$$

where A , ϕ , ψ are constants. Inserting this in (94) we have

$$(1 - \cos \phi) = -\frac{(\Delta t)^2}{\rho_0(\Delta x)^2} \left(\frac{dp}{dv} \right) \bar{v} (1 - \cos \psi) \quad (96)$$

It is well known that the factor

$$1^2 = \frac{(\Delta t)^2}{\rho_0(\Delta x)^2} \left(-\frac{dp}{dv} \right) \bar{v} \quad (97)$$

must be less than unity in order that the step-by-step solution of (90) be possible. Indeed, it is evident from (96) that if $1^2 > 1$, ϕ is imaginary near $\psi = \pi$, and hence there are disturbances which will grow exponentially with time, making the system unstable.

Otherwise, there will be N frequencies, where N is the number of space intervals in the region under consideration. The values of ψ belonging to these will be spread uniformly over the interval $-\pi$ to π .

If the linear Equation (94) were rigorous, all these oscillations would be independent. Since, however, the correct equation (90) does contain terms of higher degree, there will be a certain amount of coupling between oscillations which, given enough time, must produce some kind of statistical equilibrium.

For strong amplitudes, where the terms of different degrees in the amplitude are comparable, it is clear from dimensional arguments that the "mean free path" of the oscillations, (i.e., the distance a wave travels before equilibrium has essentially been established) that the oscillation is of the order of one interval size, with a numerical factor which, by analogy with the problem of waves in crystal lattices, one would expect to be larger than unity. As the mean amplitude is reduced and the coupling is weaker, the mean free path increases

further, and one would thus expect that for some appreciable distance behind the shock the oscillation caused by the shock may not be in equilibrium. This effect extends over a greater distance for weaker shocks.

6.5-3 Thermodynamic Relations for Small l .

We have seen above that we may expect statistical equilibrium to be established except very closely behind the shock. To this equilibrium ordinary thermodynamics is not immediately applicable, since Equation (94) is a difference equation in time as well as in space, and hence energy conservation does not hold in the usual form.

If however, $l \ll 1$, the time interval is negligible in comparison with the space interval, and the equations are then essentially differential equations in time. They are closely analogous to those for a one-dimensional Born-von Karman lattice. Since the equations are linear and there is a restoring force for each degree of freedom, it is clear that in equilibrium the thermal energy will be kT per degree of freedom, or

$$E_{th} = \frac{1}{\rho_0 \Delta x} kT \quad (98)$$

per unit mass, where $\frac{1}{\Delta x}$ is the number of degrees of freedom per unit length, k Boltzmann's constant, and T the temperature.

The unit of temperature is here arbitrary, since we cannot measure the temperature of this fictitious system by bringing it into thermal contact with any other physical system, hence only the product kT has a definite meaning. For convenience we choose our units of temperature in such a way that

$$k = \rho_0 \Delta x \quad (99)$$

or the mass per interval, hence

$$E_{th} = T \quad (100)$$

As in any other oscillating system, this energy is on the average half kinetic and half potential. Hence for the kinetic energy per unit mass

$$\frac{1}{2} \bar{u}^2 = \frac{1}{2} T$$

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or

$$\bar{u}^2 = T \quad (101)$$

where

$$u = \frac{\partial \eta}{\partial t} \quad (102)$$

is the velocity associated with the fluctuations, and the bar denotes the statistical average.

Equation (100) may be regarded as a definition of T and allows one to estimate T in any individual case. The potential energy per unit mass is

$$E(V) = \frac{1}{\rho_0} \int_V^1 p dV \quad (103)$$

For small deviations, to second order inclusive,

$$E(V) = E(\bar{V}) + \frac{1}{\rho_0} p(\bar{V})(\bar{V}-V) - \frac{1}{2} \frac{1}{\rho_0} \left(\frac{dp}{dV} \right)_{\bar{V}} (\bar{V}-V)^2 \quad (104)$$

On the statistical average, the first term gives the potential energy of the mean density without temperature, the second term vanishes, and the last represents the potential part of the thermal energy, hence:

$$\frac{1}{2\rho_0} \left(- \frac{dp}{dV} \right)_{\bar{V}} \overline{(\bar{V}-V)^2} = \frac{1}{2} T \quad (105)$$

or

$$\overline{(\bar{V}-V)^2} = \rho_0 T \left| \frac{dp}{dV} \right|^{-1} \quad (106)$$

Since $\frac{dp}{dV}$ is known and T can be found from (101), this relation can be treated. However, the equality of kinetic and potential energy, in the time average, holds for any harmonic motion whether in equilibrium or not. Hence this test merely verifies that the amplitudes of oscillation are weak enough to make the motion essentially harmonic.

We can now find the pressure caused by the heat motion. By expansion to second order

$$p = p(\bar{V}) + \frac{dp}{dV} (V-\bar{V}) + \frac{1}{2} \frac{d^2 p}{dV^2} (V-\bar{V})^2 \quad (107)$$

On the average, the first term is the pressure due to the mean density without

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temperature, the second term vanishes; the last is the thermal pressure. Hence

$$P_{th} = \frac{1}{2} \left[\frac{d^2 p}{dV^2} \right]_{\bar{V}} (\bar{V} - V)^2 = -\frac{1}{2} (\bar{V} - V)^2 \frac{d}{dV} \left| \frac{dp}{dV} \right| \quad (108)$$

(The negative sign comes from the fact that $\frac{dp}{dV}$ is necessarily negative.)

Using (106)

$$P_{th} = -\frac{1}{2} \rho_0 T \frac{d}{dV} \left(\log \left| \frac{dp}{dV} \right| \right) \quad (109)$$

The same relation can be derived in a different way. In general

$$p = - \frac{\partial F}{\partial v} = - \rho_0 \frac{\partial F}{\partial V} \quad (110)$$

where F is the free energy per unit mass, and v the volume per unit mass.

F is a sum over the different degrees of freedom, and for each degree of freedom,

$$F_i = -kT \log W_i + \text{const.} \quad (111)$$

where W_i is its frequency (in radians per second) and the constant may depend on the temperature but not on V . Hence, using (99)

$$P_{th} = - \frac{\rho_0^2 T \Delta x}{M} \sum_i \frac{\partial \log W_i}{\partial V} \quad (112)$$

the sum to extend over all degrees of freedom belonging to the region considered, which has a total mass M . The frequencies are to be found from (96) with

$$W = \frac{1}{\Delta t} \phi \quad (113)$$

If ϕ is small, the right-hand side of (96) is always small, hence ϕ is a small angle and the left-hand side can be replaced by $\frac{1}{2} \phi^2$. Hence each of the frequencies is proportional to $\sqrt{\left| \frac{dp}{dV} \right|}$ and

$$W_i = f_i \sqrt{\left| \frac{dp}{dV} \right|} \quad (114)$$

where f_i depends on the wave number k_i , but not on V . Hence all terms of the sum in (112) are equal, and the number of terms is equal to the number of intervals in a mass M , i. e., to

.

$$\frac{M}{\rho_0 \Delta x}$$

(115)

Inserting this in (112) we obtain again (109)

This derivation is of interest since it shows the dependence of the result on the relation (114), which is not correct unless l is small.

We may reasonably surmise that, for our present purpose, l can be regarded as small as long as (114) is substantially correct. To test this, the solutions of (96) have been plotted in Figure 18 against l for different angles ϕ . It is seen that all lines are straight in good approximation up to $l = \frac{1}{2}$ and in view of (97) this means that in this range all frequencies are proportional to $\sqrt{\left| \frac{dp}{dV} \right|}$. For $l = \frac{1}{2}$ only the uppermost curves begin to bend, and without further investigation it is not possible to estimate to what extent this would affect our conclusions.

6.5-4 Hugoniot Relations.

Consider now a shock running into material at rest. (This causes no essential loss of generality.) Let V_1 be the specific volume, p_1 the pressure ahead of the shock, and assume there is no thermal motion ahead of the shock. Then the first Hugoniot relation is

$$\bar{u} = U(1 - \bar{V}/V_1) \tag{116}$$

where \bar{u} is the mean velocity and \bar{V} the mean specific volume behind the shock, U the shock velocity. This relation only expresses conservation of material and must be satisfied automatically in our model.

The other two relations:

$$p - p_1 = \rho_0 U^2 \frac{V_1 - \bar{V}}{V_1^2} \tag{117}$$

and

$$\rho_0 (E - E_1) = \frac{1}{2} (V_1 - \bar{V})(p + p_1) \tag{118}$$

will now also contain the thermal pressure and energy:

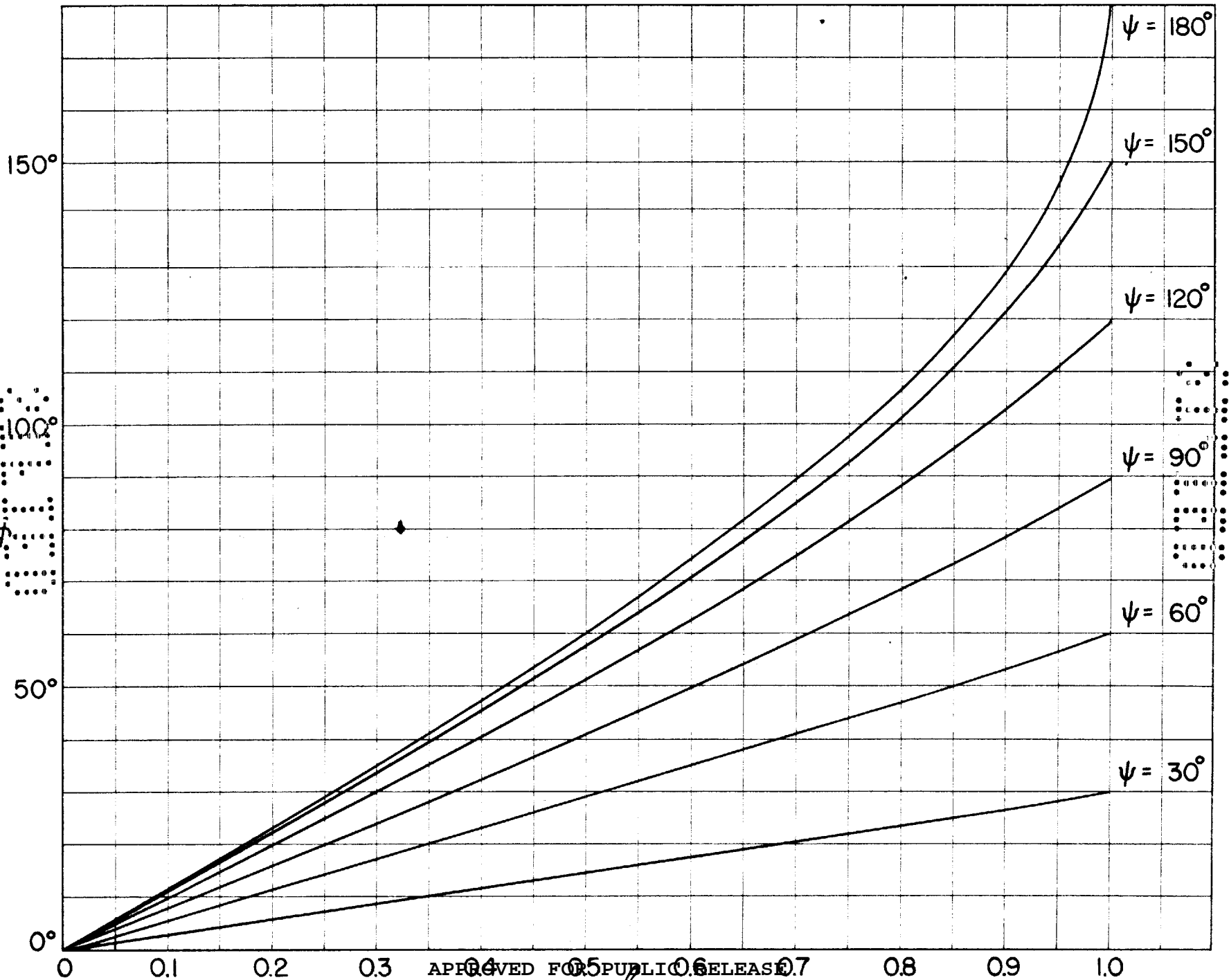
$$p(\bar{V}) - p_1 + p_{th} = \frac{\rho_0 U^2}{V_1^2} (V_1 - \bar{V}) \tag{119}$$

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Figure 18

Frequency as function of l for varying
ratio of wavelength to spacing

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$$\rho_0 [E(\bar{V}) - E_1 + E_{th}] = \frac{1}{2} [p(\bar{V}) - p_1 + p_{th}] (V_1 - \bar{V}) \quad (120)$$

It is convenient to write g for the ratio

$$g = \rho_0 \frac{E_{th}}{p_{th}} \quad (121)$$

Then, by (100) and (109):

$$g = \frac{2}{\left| \frac{d}{dV} \log \left| \frac{dp}{dV} \right| \right|} \quad (122)$$

and with this abbreviation, we can solve (120) for p_{th} :

$$p_{th} = \frac{\frac{1}{2} (p+p_1)(V_1-\bar{V}) - \rho_0 [E(\bar{V}) - E_1]}{g - \frac{1}{2} (V_1-\bar{V})} \quad (123)$$

and

$$\frac{\rho_0 v^2 (V_1-\bar{V})}{v_1^2} = \frac{g [p(\bar{V}) - p_1] + p_1 (V_1-\bar{V}) - \rho_0 [E(\bar{V}) - E_1]}{g - \frac{1}{2} (V_1-\bar{V})} \quad (124)$$

The thermodynamic properties of the model are unimportant as long as (123) is small compared to the pressure $p(\bar{V})$. At the same time (123) allows one to estimate the amplitude of the fluctuations to be expected behind a shock of given strength.

For this purpose one may either compare the average pressure with the pressure belonging to the average volume \bar{V} or use the mean square velocity fluctuation, which, using (121) and (100) (101), is

$$\overline{u_{th}^2} = g p_{th} \quad (125)$$

For strong shocks it is evident from (123) that there is a limiting compression ratio which cannot be exceeded even for an infinite pressure, and this is given by the condition

$$g = \frac{1}{2} (V_1 - \bar{V}) \quad (126)$$

As g depends on the volume in the final state, it is most convenient to express the limiting compression by giving the highest volume V_1 for which a given \bar{V} can be reached in a single shock:

$$V_1 = \bar{V} + 2g \cdot (\bar{V}) \quad (127)$$

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Figure 19 shows g as a function of the specific volume \bar{V} for air, and the limiting volume V_1 for which a given \bar{V} can be reached.

Figure 20 shows the thermal pressure for air, starting at normal volume. For comparison, the "cold" pressure, $P(V)$, and the correct thermal pressure, as calculated by Keller, are also shown.

It is evident from this figure that, whenever the thermal pressure amounts to an appreciable contribution to the cold pressure, it is considerably in excess of the true value.

Table 6.5-4 lists the thermal pressures for air for various values of V_1 and \bar{V} .

From these values, the mean amplitude of the fluctuations was obtained by the formula

$$\overline{\Delta V^2} = P_{th} g \left| \frac{dp}{dV} \right|^{-1} \quad (128)$$

which follows immediately from (106), (100) and (121). Since for a harmonic oscillation the root mean square amplitude is $\frac{1}{\sqrt{2}}$ times the maximum amplitude, we can define a minimum volume that would be reached for harmonic oscillation of the same $\overline{\Delta V^2}$. This is

$$V_{min} = \bar{V} - \sqrt{2 \overline{\Delta V^2}} \quad (129)$$

See Table 6.5-1.

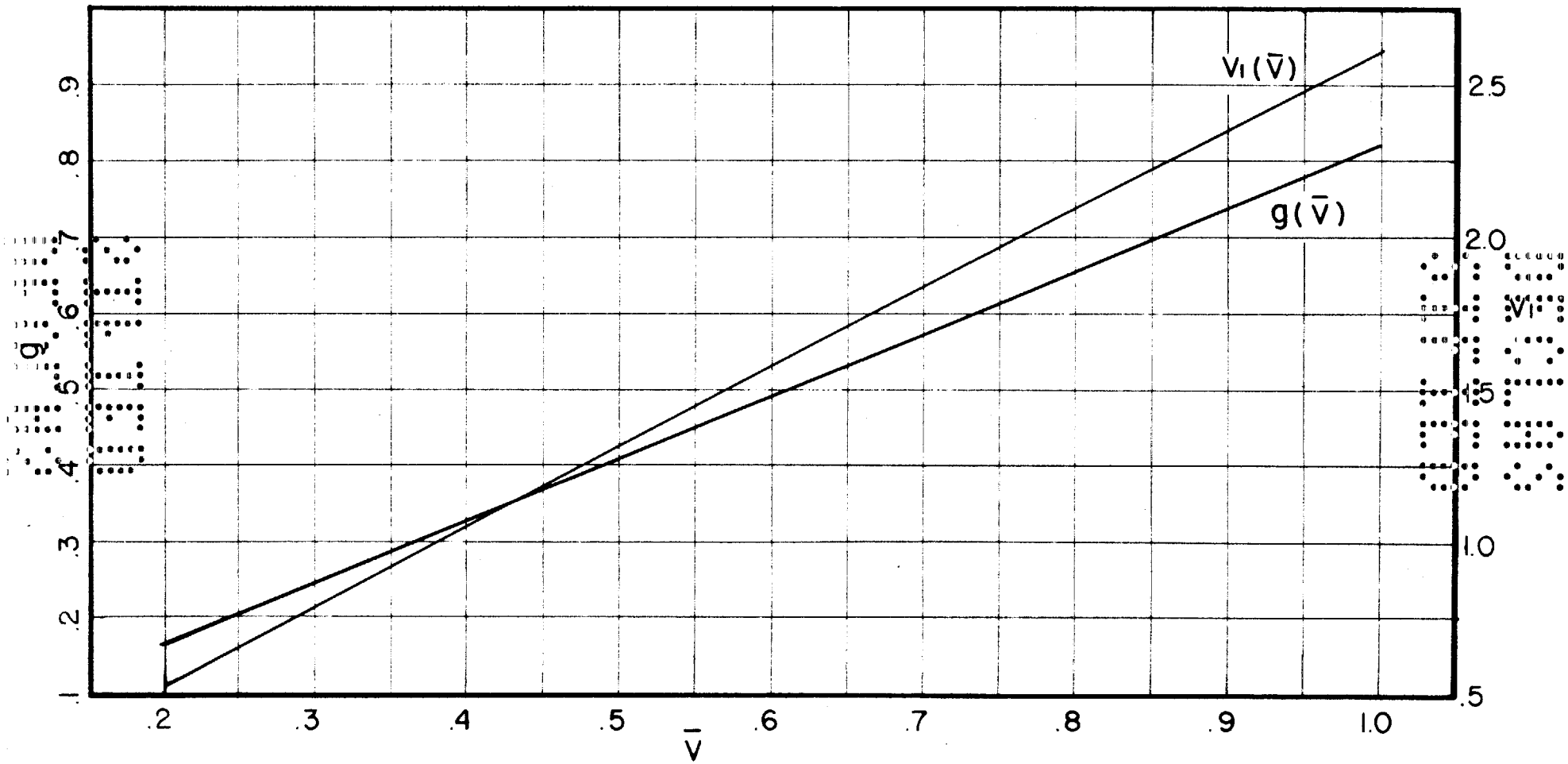
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Figure 19

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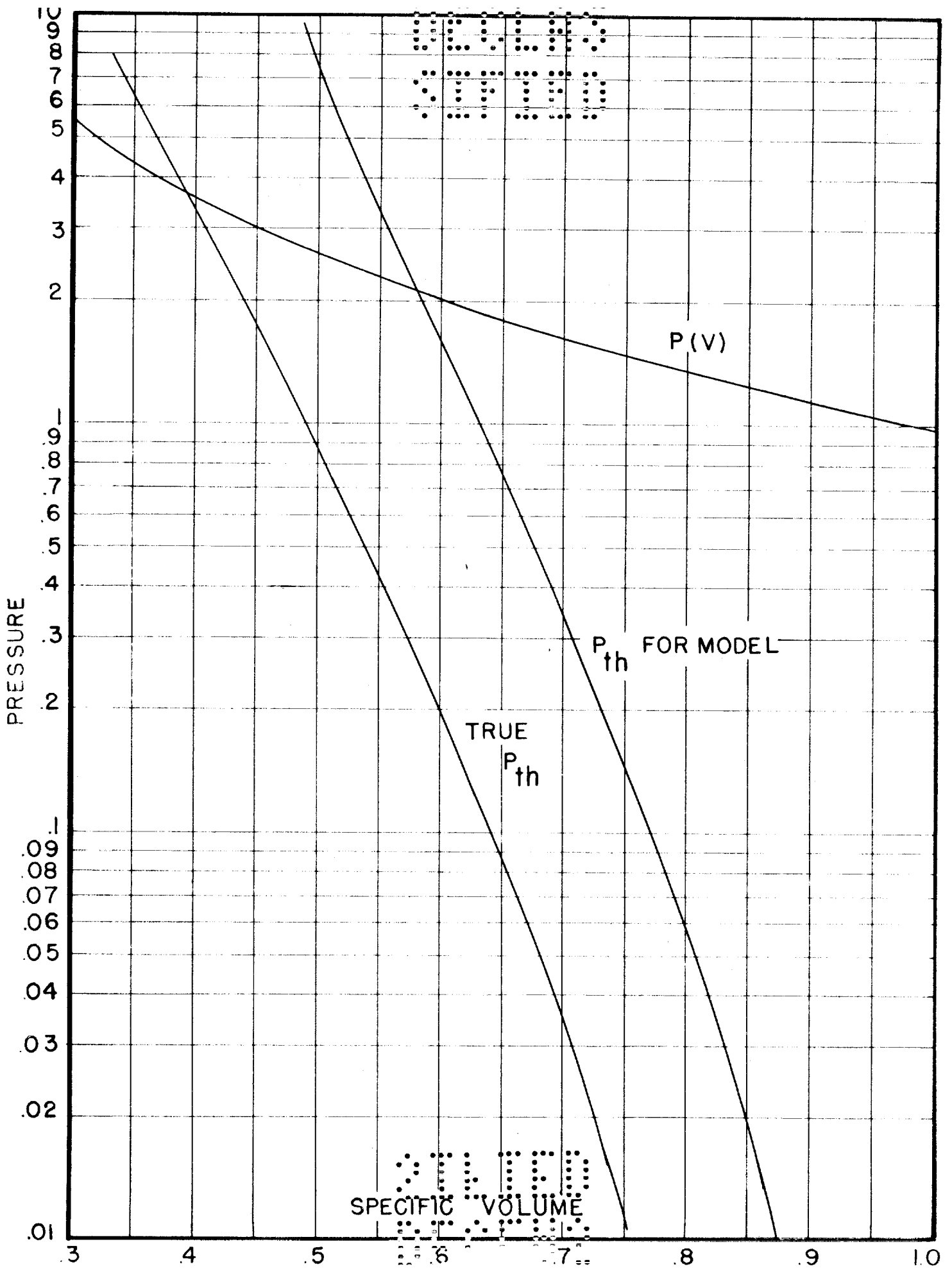
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Figure 20

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Table 8.5-4

$P_{th}(V_1, \bar{V})$

$V_1 \backslash \bar{V}$.80	.70	.60	.50	.40	.30	.20
1.0	.0057	.0333	.1484	.7207	10.905		
.90	.0007	.0107	.0643	.3387	2.6251		
.80	0	.0018	.0207	.1425	1.004		
.70		0	.0027	.0446	.3849	5.873	
.60			0	.0064	.1173	1.532	
.50				0	.0170	.4099	32.20
.40					0	.0550	2.796
.30						0	.3252
.20							0

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6.5-5 Other Effects.

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The analysis given in the previous sections is in some ways still very idealized, and we want to discuss a few effects that have been neglected.

- (1) The fact has already been referred to that the discussion applies only to small l , and probably in practice to $l < l/2$. This probably covers all applications of practical interest.
- (2) Moreover, we have assumed that the oscillations are always in statistical equilibrium. In fact, all oscillations arise at the shock front, and it will take them a finite time to get into equilibrium. This means that there will be a region behind the shock front in which there is no equilibrium. The extent of this region is inversely proportional to the temperature, since the establishment of equilibrium depends on the coupling between different degrees of freedom by the terms of higher order in the amplitude of the oscillations. This effect may cause errors if the extent of the non-equilibrium region is comparable to the distance over which the dynamical variables change appreciably.
- (3) In the discussion given above, we have assumed harmonic oscillations, which is correct only for small amplitudes. When the "thermal" pressure exceeds the "cold" pressure this is no longer justified. As a result the thermodynamic properties of the system may differ from our description at high temperatures, and in particular the limiting compression may be appreciably affected. On the other hand the limit of applicability of the method will remain unchanged since this refers to the condition that the thermal pressure is negligible, which means that it must have small amplitude.
- (4) Conduction of energy. In the physical applications of most interest heat conduction is usually negligible, and an accurate model therefore ought to give adiabatic changes in the state of matter everywhere except

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at the shock front. In our model there exists a finite heat conductivity carried by the sound waves and limited mainly by the second-order terms which limit the free run of such waves. The "mean free path" of the waves is dimensionally of the order of the interval size, multiplied by a function of temperature which is large for low temperatures. Hence, one may expect some error due to this effect for weak shocks. However, as the heat content is then small, this will not lead to appreciable errors. In any case, for any shock strength this effect can be made negligible by a generous choice of the number of intervals used.

(5) Changing interval size. It is often convenient in calculations not to make all intervals equal but to use groups of smaller intervals in regions where more structure is required. Consider the boundary between two such groups. Physically, the two parts of the material ought to be in equilibrium for equal temperature, i.e., for equal energy per unit mass. However, in the model this does not correspond to equality of temperatures as defined by (100) since the latter is measured on a conventional scale. In the model, the two groups of points are in equilibrium if the energy per degree of freedom is the same, which means different energies per unit mass. What we have done corresponds, in effect, to using different values of Avogadro's number in different parts of the material.

Suppose, for example, that a shock is moving through a range where the interval size is Δx , and that a short distance behind the shock it is reduced to $\Delta x/2$. Then, as soon as the disturbances have had time to travel back to the region with the smaller intervals, an equilibrium will be approached in which the energy per interval is the same, so that the temperature at the small intervals will be twice as high as in the larger ones.

6.5-6 Application to Spherical Problems.

An important class of problems concerns motion with spherical symmetry. Then we have, in place of (89).

$$\frac{\partial^2 R}{\partial t^2} = -\frac{1}{\rho_0} \frac{R^2}{r^2} \frac{dP}{dV} \frac{\partial^2 \eta}{\partial r^2} \quad (130)$$

where R is the actual distance from the center, and the independent variable r is the original distance between the point considered and the center. If we are to obtain the linear equations for small disturbances, we must bear in mind that the mass contribution to the free energy comes from oscillations with wave lengths of the order of the interval size, and that, for any reasonable choice of interval, this is small compared to the distance from the center. Hence if we write again

$$R = \bar{R} + \eta \quad (131)$$

where \bar{R} represents the undisturbed motion, the variation of η is much more rapid than that of \bar{R} . Hence we find:

$$\ddot{\eta} = -\frac{1}{\rho_0} \frac{R^2}{r^2} \frac{dP}{dV} \frac{R^2}{r^2} \frac{\partial^2 \eta}{\partial r^2} \quad (132)$$

Here $\frac{R^2}{r^2}$ should be regarded as locally constant. If the calculation is carried out with constant intervals in radius, this leads to an equation of the type of (94). It is still true that upon a change in volume each frequency is proportional to $\sqrt{\frac{dp}{dV}}$ and hence the formulae of Section 6.5-3 still apply.

However, in addition, the frequencies vary with R , the position of the radial element, and thus we find a dependence of free energy on position. This means a radial force G per unit mass.

$$G = - \frac{\partial F}{\partial R} \quad (133)$$

Using (111)

$$G = \frac{\rho_0 \Delta x}{M} T \sum_1 \frac{\partial \log W_1}{\partial R} \quad (134)$$

and, in view of (132)

$$\frac{\partial \log W_1}{\partial R} = \frac{2}{R}$$

so that

$$G = - \frac{2T}{R} \quad (135)$$

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Using (121) and (100):

$$G = - \frac{2g}{R\rho_0} P_{th} \quad (136)$$

If g is near $1/2$, which is the case for a considerable range of values of \bar{V} for air,

$$\rho_0 G = - P_{th}/R \quad (137)$$

If the true pressure varies, for example, as the inverse radius, the true pressure gradient is $-\frac{P}{R}$, and thus the relative error in the acceleration is of the order of P_{th}/P , i.e., the same as the relative error in the pressure itself.

6.5-7 Comparison with I.B.M. Calculations.

In the I.B.M. solution of the problem of a spherical blast wave, the von Neumann method of treating the shock was not used; conditions at the shock front were treated separately by the Hugoniot relations, which gave data to be used as boundary conditions in the I.B.M. solution. However, another problem, that of a plane blast wave in air, was treated by the von Neumann method. One would expect that this problem would give quite clean-cut results, since there is no change in interval size and there are none of the effects of the radial problem.

Figure 22 shows, for three mass points, the specific volume as a function of time. Since the period of this oscillation is considerably larger than one time interval, the curves show the motion quite clearly; for the dynamical quantities at fixed time, the period is of the order of one mass interval, and the curves are not clear. It is clear that the motion is fairly harmonic; the first minimum thus should represent the mean volume of the shocked material minus the maximum amplitude of the shock, and the curves of Figure 21 should be applicable. We get:

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Mass point no	2.5	3.5	4.5
V_1	1.0	1.0	1.0
V_{min}	.555	.535	.515
\bar{V}	.673	.663	.650

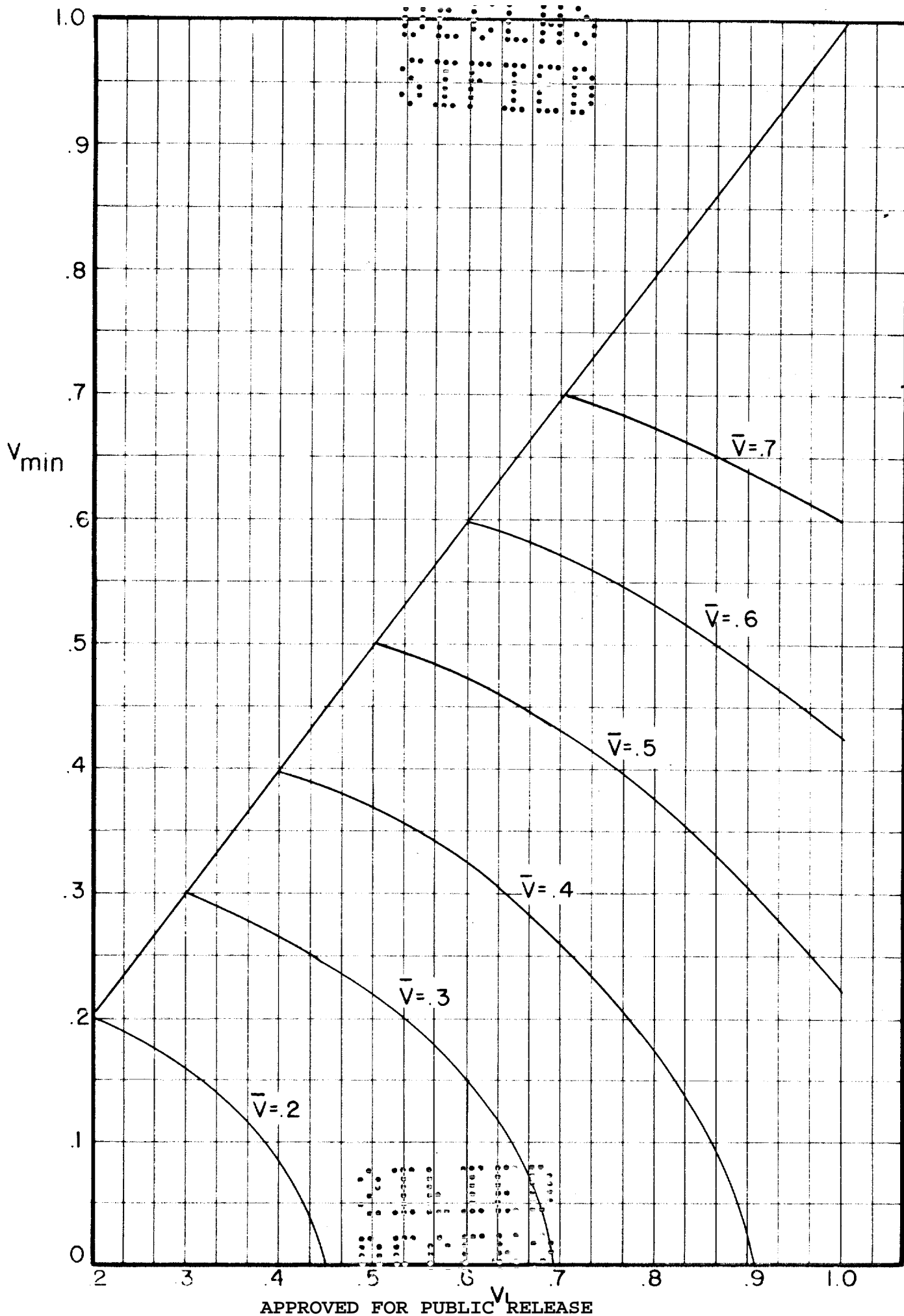
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Figure 21

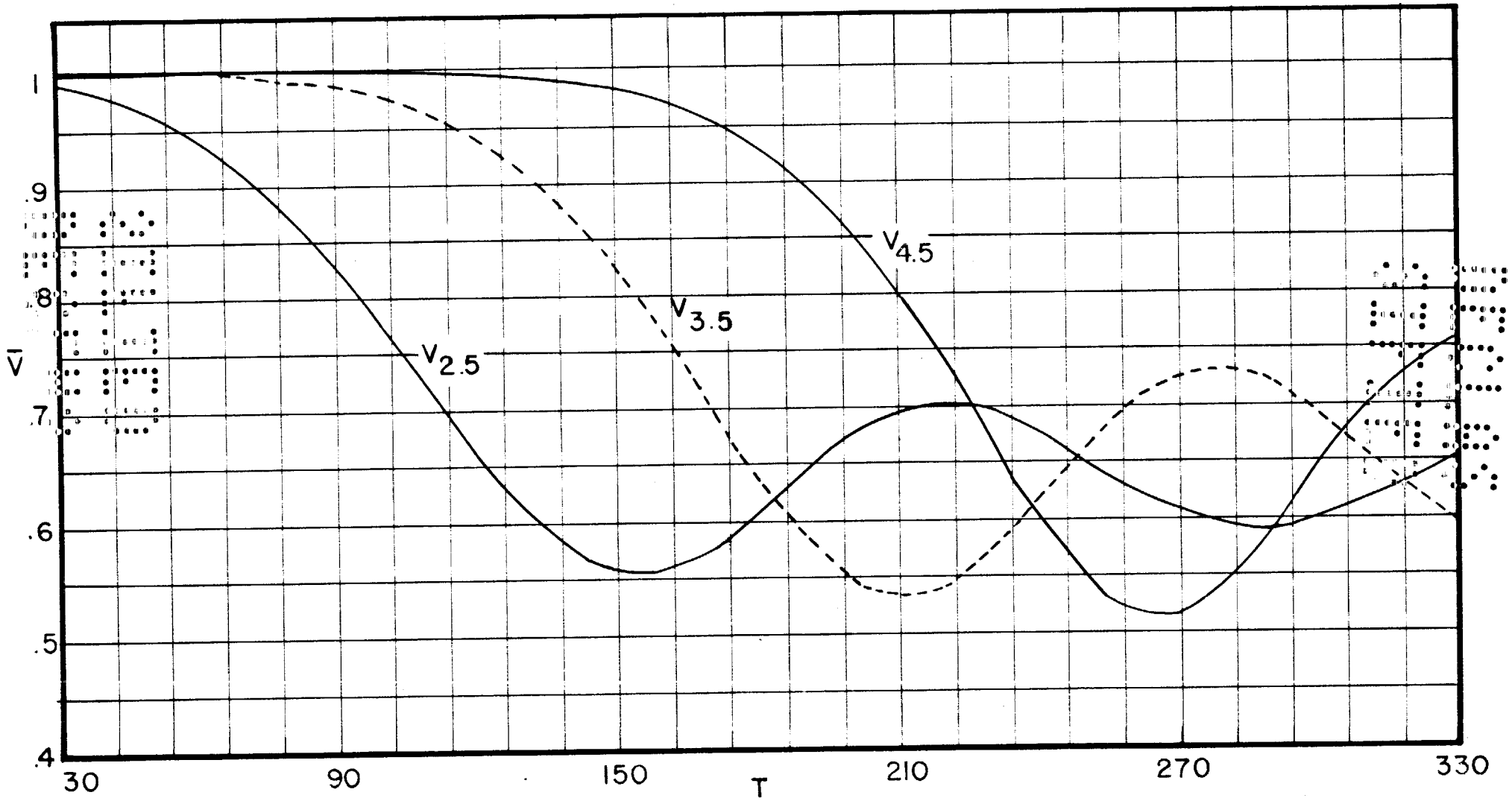
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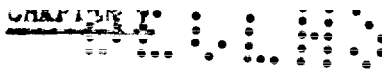


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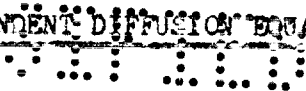
Figure 22

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SOLUTION OF THE TIME DEPENDENT DIFFUSION EQUATION



S. Goldberg and J. Kemeny

7.1 MATHEMATICAL FORMULATION OF THE PROBLEM

If one considers a system of particles moving in a material which both absorbs and scatters, the distribution of these particles in space and time is given by the Boltzmann Equation:

$$\frac{\partial n(r, \mu, t)}{\partial t} + v \cdot \nabla n(r, \mu, t) = -\sigma v n(r, \mu, t) + \frac{\sigma v(1+f)}{2} \int_{-1}^{+1} n(r, \mu', t) d\mu' \quad (1)$$

where

$n(r, \mu, t)$ = number of particles (per unit volume) at point r , at time t , moving in the direction given by the direction cosine μ made with the radius vector,

v = velocity of the particles,

σ = the collision probability per unit path of length,

$1+f$ = the mean number of particles emerging per collision.

As an example of a problem to which this equation is applicable, consider the following: A known distribution of neutrons is introduced into the system. Depending upon the geometry and material construction of this system, the neutron distribution will grow or decay in time. (Provided that the distribution is not stationary.) The Boltzmann Equation (1) describes the growth of such a neutron population. The asymptotic solution for (1) shows that the population grows as $e^{\alpha t}$. We want to find α .

We must first reduce equation (1) to a form more suitable for numerical solution. To do this consider the gradient in (1) taken along a given direction described by the coordinate q . The equation then reads

$$\frac{\partial n(r, \mu, t)}{\partial t} + v \frac{\partial n(r, \mu, t)}{\partial q} = -\sigma v n(r, \mu, t) + \frac{\sigma v(1+f)}{2} \int_{-1}^{+1} n(r, \mu', t) d\mu' \quad (i)$$

We now make substitutions

$$z = \frac{q+vt}{2}$$

$$y = \frac{q-vt}{2}$$



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so that

$$\frac{\partial n}{\partial q} \rightarrow \frac{1}{2} \left[\frac{\partial n}{\partial \xi} + \frac{\partial n}{\partial \eta} \right], \quad \frac{\partial n}{\partial t} \rightarrow \frac{1}{2} v \left[\frac{\partial n}{\partial \xi} + \frac{\partial n}{\partial \eta} \right]$$

Equation (1') now becomes

$$\frac{\partial n(r, \mu, t)}{\partial \xi} + \sigma n(r, \mu, t) = \frac{\sigma(1+f)}{2} \int_{-1}^{+1} n(r, \mu', t) d\mu' \quad (2)$$

if we now multiply both sides of this equation by $e^{\sigma \xi}$, we may rewrite it in the form

$$\frac{\partial}{\partial \xi} \left[n(r, \mu, t) e^{\sigma \xi} \right] = \frac{\sigma(1+f)}{2} e^{\sigma \xi} \int_{-1}^{+1} n(r, \mu', t) d\mu' \quad (2')$$

Integrating along the direction ξ from initial point ξ_0 to a final point ξ , we get

$$n(\xi) e^{\sigma \xi} - n(\xi_0) e^{\sigma \xi_0} = \int_{\xi_0}^{\xi} \frac{\sigma(1+f)}{2} e^{\sigma \xi'} \int_{-1}^{+1} n(r, \mu', t) d\mu' d\xi'$$

and rewriting gives

$$n(\xi) = n(\xi_0) e^{-\sigma(\xi-\xi_0)} + \int_{\xi_0}^{\xi} \frac{\sigma(1+f)}{2} e^{-\sigma(\xi-\xi')} \int_{-1}^{+1} n(r, \mu', t) d\mu' d\xi' \quad (3)$$

Now if we let ξ refer to time t , ξ_0 to time $t - \Delta t$, then

$$\xi - \xi_0 = \frac{v + vt}{2} - \frac{v - v\Delta t + v(t - \Delta t)}{2} = v\Delta t$$

$v \Delta t$ is of course the distance the particle travels in a given direction in time Δt , provided that it suffers no collisions. Under the transformation

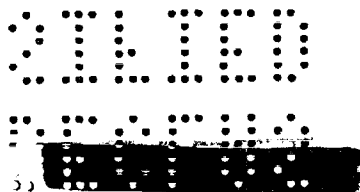
$$\xi - \xi' = s v \Delta t,$$

equation (3) becomes

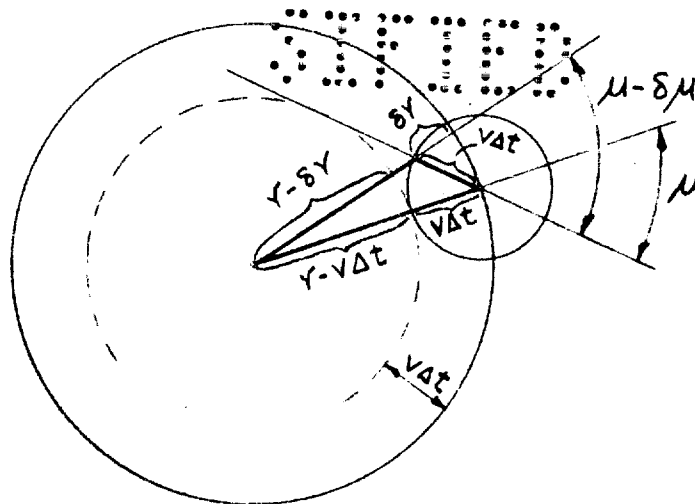
$$n(r, \mu, t) = n(r - \delta r, \mu - \delta \mu, t - \Delta t) e^{-\sigma v \Delta t} + \int_0^1 \frac{\sigma(1+f)}{2} v \Delta t ds \int_{-1}^{+1} d\mu' e^{-\sigma v s \Delta t} n(r - s \delta r, \mu', t - s \Delta t) \quad (4)$$

Equation (4) is now in the form which can easily be transformed for numerical computation. We want to treat this as a two-dimensional problem; therefore, we shall assume spherical symmetry.

We must first fix intervals in space (Δr), in angle ($\Delta \mu$), and in time (Δt). The details of this procedure will be outlined in section 7.3. δr and $\delta \mu$ are then functions of r, μ , and these interval values. We can easily find these expressions with the aid of the following diagram. Our problem is spherically symmetric so that we need consider our equation along one radius only.



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An application of the law of cosines and the law of sines to the triangle indicated yields the equations

$$(v - \delta r)^2 = r^2 + (v \Delta t)^2 - 2rv \Delta t \mu,$$

$$\frac{\sqrt{1 - \mu^2}}{r - \delta v} = \frac{\sqrt{1 - (\mu - \delta \mu)^2}}{r}$$

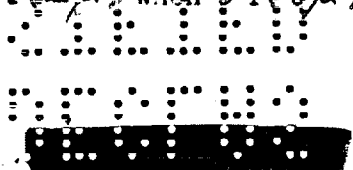
One may easily verify algebraically that δr and $\delta \mu$ are given by the following formulae:

$$\delta r = r - R, \quad \delta \mu = \mu - \frac{1}{R} (\mu r - v \Delta t) \quad (5)$$

where

$$R = \sqrt{r^2 + (v \Delta t)^2 - 2rv \Delta t \mu}$$

It must be remembered that I.B.M. machines can perform arithmetical operations only, and therefore we must make further simplifying assumptions to be able to carry out the operations indicated in (4). We first assume that the term $n(r - \delta r, \mu - \delta \mu, t - \Delta t)$ is a linear combination of $n(r, \mu, t - \Delta t)$, $n(r, \mu \pm \Delta \mu, t - \Delta t)$, $n(r \pm \Delta r, \mu, t - \Delta t)$ and $n(r \pm \Delta r, \mu \pm \Delta \mu, t - \Delta t)$. Here, as in the following paragraphs, the + or - sign is adjusted so that we should always get an interpolation, not an extrapolation formula. That is the + sign goes with $\Delta r (\Delta \mu)$ when $\delta r (\delta \mu)$ is negative, the - sign goes with $\Delta r (\Delta \mu)$ when $\delta r (\delta \mu)$ is positive. Now



$$n(r, \mu - \delta\mu, t - \Delta t) = \frac{1}{\Delta\mu} \left[|\delta\mu| n(r, \mu \pm \Delta\mu, t - \Delta t) + (\Delta\mu - |\delta\mu|) n(r, \mu, t - \Delta t) \right]$$

and

$$n(r - \delta r, \mu - \delta\mu, t - \Delta t) = \frac{1}{\Delta r} \left[|\delta r| n(r \pm \Delta r, \mu - \delta\mu, t - \Delta t) + (\Delta r - |\delta r|) n(r, \mu - \delta\mu, t - \Delta t) \right]$$

Using these two interpolation formulae one easily derives the final equation:

$$n(r - \delta r, \mu - \delta\mu, t - \Delta t) = \frac{|\delta r \delta \mu|}{\Delta r \Delta \mu} n(r \pm \Delta r, \mu \pm \Delta \mu, t - \Delta t) + \frac{|\delta r| (\Delta \mu - |\delta \mu|)}{\Delta r \Delta \mu} n(r \pm \Delta r, \mu, t - \Delta t) + \frac{(\Delta r - |\delta r|) |\delta \mu|}{\Delta r \Delta \mu} n(r, \mu \pm \Delta \mu, t - \Delta t) + \frac{(\Delta r - |\delta r|) (\Delta \mu - |\delta \mu|)}{\Delta r \Delta \mu} n(r, \mu, t - \Delta t) \quad (6)$$

Having chosen the radii and angle values and intervals $\Delta r, \Delta \mu, \Delta t$, the four coefficients above are fixed constants for given r and μ . Since we assume that the density remains constant, σ is a known constant in any particular material. Since $e^{-\sigma v \Delta t}$ is a constant for the problem, the evaluation of the term $n(r - \delta r, \mu - \delta \mu, t - \Delta t) e^{-\sigma v \Delta t}$ in equation (4) is reduced to finding the sum of four products. Equation (4) now has the form:

$$n(r, \mu, t) = a_1 n(r \pm \Delta r, \mu \pm \Delta \mu, t - \Delta t) + a_2 n(r \pm \Delta r, \mu, t - \Delta t) + a_3 n(r, \mu \pm \Delta \mu, t - \Delta t) + a_4 n(r, \mu, t - \Delta t) + \frac{\sigma(1+f)}{2} v \Delta t \int_0^1 ds \int_{-1}^1 d\mu' n(r - s\delta r, \mu', t - s\Delta t) e^{-\sigma v \Delta t s} \quad (7)$$

where the a_i are the coefficients in (6), each multiplied by $e^{-\sigma v \Delta t}$.

We turn now to the simplification of the last term in (7) involving two integrations, with respect to μ and then with respect to the auxiliary variable s . We denote the integral $\int_{-1}^1 n(r - s\delta r, \mu', t - s\Delta t) d\mu'$ by

$$\bar{n}(r - s\delta r, t - s\Delta t). \text{ In order to evaluate } \int_0^1 \bar{n}(r - s\delta r, t - s\Delta t) e^{-\sigma v \Delta t s} ds \quad (8)$$

we assume that $\bar{n}(r, t)$ varies linearly in r and t . Then the integral (8) becomes a linear combination of $\bar{n}(r, t)$, $\bar{n}(r \pm \Delta r, t)$, $\bar{n}(r, t - \Delta t)$, and $\bar{n}(r \pm \Delta r, t - \Delta t)$. Just as we derived the interpolation formula (6), we can similarly demonstrate that

$$\bar{n}(r - s\delta r, t - s\Delta t) = (1-s)(1-s \frac{|\delta r|}{\Delta r}) \bar{n}(r, t) + s(1-s) \frac{|\delta r|}{\Delta r} \bar{n}(r \pm \Delta r, t) + s(1-s) \frac{|\delta r|}{\Delta r} \bar{n}(r, t - \Delta t) + s^2 \frac{|\delta r|}{\Delta r} \bar{n}(r \pm \Delta r, t - \Delta t) \quad (9)$$

One may easily verify the following formula:

$$\int_0^1 (As^2 + Bs + C) e^{-\sigma v \Delta t s} ds = A \left[\frac{1 - e^{-\sigma v \Delta t}}{(\sigma v \Delta t)^2} + \frac{1 - e^{-\sigma v \Delta t}}{(\sigma v \Delta t)^3} \right] + B \left[-\frac{e^{-\sigma v \Delta t}}{\sigma v \Delta t} + \frac{1 - e^{-\sigma v \Delta t}}{(\sigma v \Delta t)^2} \right] + C \left[\frac{1 - e^{-\sigma v \Delta t}}{\sigma v \Delta t} \right]$$

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We may use this general integration formula to integrate (8) after substituting (9) for $\bar{n}(Y-5\delta Y, t-5\Delta t)$. This reduces the last term in (7) to exactly the same form as the first part, i.e., to the sum of four simple products. Equation (4) now has the convenient form:

$$n(r, \mu, t) = a_1 n(r \pm \Delta r, \mu \pm \Delta \mu, t - \Delta t) + a_2 n(r \pm \Delta r, \mu, t - \Delta t) + a_3 n(r, \mu \pm \Delta \mu, t - \Delta t) + a_4 n(r, \mu, t - \Delta t) + a_5 \bar{n}(r, t) + a_6 \bar{n}(r \pm \Delta r, t) + a_7 \bar{n}(r, t - \Delta t) + a_8 \bar{n}(r \pm \Delta r, t - \Delta t) \quad (10)$$

For the exact value of the a_i see Section 7.3.

There remains one further problem. Equation (10) tells us that in order to get $n(r, \mu, t)$ we must know n at $t - \Delta t$, and \bar{n} at t and $t - \Delta t$. In the problem as stated above we have n and \bar{n} at $t - \Delta t$, but we do not have \bar{n} at t . (i.e., we know the distribution up to time $t - \Delta t$, but we have yet to find it for t .) Finding it for t is precisely our problem. We have to make the further assumption that \bar{n} grows exponentially in time at a given radius, i.e.,

$$\frac{\bar{n}(r, t)}{\bar{n}(r, t - \Delta t)} = e^{\gamma \Delta t}$$

It is then easy to see that $\bar{n}(r, t)$ may be expressed in terms of known quantities as follows:

$$\bar{n}(r, t) = \frac{[\bar{n}(r, t - \Delta t)]^2}{\bar{n}(r, t - 2\Delta t)}$$

In the following sections a detailed description will be given of the I.B.M. method used in solving Equation (10).

7.2 I.B.M. PROCEDURE. GENERAL OUTLINE

Our problem presents itself to us in the form of given distributions $n(r, \mu, t)$, $\bar{n}(r, t - \Delta t)$, and $\bar{n}(r, t)$, from which we have to calculate $n(r, \mu, t + \Delta t)$ and $\bar{n}(r, t + \Delta t)$ by the use of the following formulae:

.



$$n(r, \mu, t + \Delta t) = a_1 n(r \pm \Delta r, \mu \pm \Delta \mu, t) + a_2 \bar{n}(r \pm \Delta r, \mu, t) + a_3 n(r, \mu \pm \Delta \mu, t) + a_4 n(r, \mu, t) + a_5 \bar{n}(r, t + \Delta t) + a_6 \bar{n}(r \pm \Delta r, t + \Delta t) + a_7 \bar{n}(r, t) + a_8 \bar{n}(r \pm \Delta r, t)$$

$$\bar{n}(r, t + \Delta t) = \int_{\mu_1}^{\mu_2} n(r, \mu, t + \Delta t) d\mu$$

where a_1 are the functions of r and μ only, and the \pm signs are fixed for each r, μ .

All the quantities up to time t are known, but we do not have $\bar{n}(t + \Delta t)$.

As stated previously, we assume that

$$\bar{n}(t + \Delta t) = \frac{[\bar{n}(t)]^2}{\bar{n}(t - \Delta t)}$$

Therefore we start out by squaring $\bar{n}(t)$, and then we divide the square by

$\bar{n}(t - \Delta t)$. (The deck containing these \bar{n} 's has only one card for each r ;

hence, it is known as the small deck. The large deck contains the n 's, having one card for every combination of r and μ .) After the small deck has gone

through operations 1 and 2, we have all the needed n 's and \bar{n} 's, and we have

to multiply them by the fixed a_1 's. Whenever there is a problem involving

a large number of multiplications in each of which there is a factor that does

not change from one cycle to the other, the masterdeck method can be used

to great advantage. (This method was also used in matrix-multiplication,

which is described in another chapter of this volume.)

From the equation for $n(r, \mu, t + \Delta t)$ we see that a particular $n(r, \mu, t)$

may be used for the computation of several of the $n(r, \mu, t + \Delta t)$, $n(r \pm \Delta r,$

$\mu \pm \Delta \mu, t + \Delta t)$, etc. Therefore, $n(r, \mu, t)$ is multiplied by several different

a_1 . The simplest way of handling this is to use $n(r, \mu, t)$ as a group-

multiplier for these a_1 . These a_1 do not change, and the same a_1 are always

multiplied by the same n 's. Therefore, we make up a masterdeck in which each

card has an $a_1(r', \mu')$ and which has the r of the n which will multiply the

a_1 . Then we can combine the masterdeck (a_1 - a_4) sorting on r and μ . We put

the combined deck through the multiplier, punching $a_1 n$ on each mastercard.

A similar procedure is followed for the small deck with the \bar{n} 's. The master-

deck is then re-sorted on r' and μ' (so that the eight products whose sum



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is $n(r', \mu')$ follow each other), and the products are summed.

It is very important to understand the difference between r, μ and r', μ' . To every a_i corresponds an r and an r' ; to $a_i (i=1, \dots, 4)$ correspond an r' and a μ' also. That is, if

$$n(r_0, \mu_0, t + \Delta t) = a_1 n(r_0 - \Delta r, \mu_0 + \Delta \mu, t) + \dots + a_8 \bar{n}(r_0 - \Delta r, t)$$

then $r' = r_0$, $\mu' = \mu_0$, $r = r_0 - \Delta r$, $\mu = \mu_0 + \Delta \mu$

Hence, during multiplication r, μ are important, while during the summing of the products r', μ' become significant.

The products are added up in the tabulator, and at the same time a new large deck is summary punched. This new deck contains the n 's on which we have to perform an integration:

$$\bar{n}(r, t + \Delta t) = \int_{-1}^{+1} n(r, \mu, t) d\mu$$

For any given r , $\Delta \mu$ is constant (we choose equal intervals in μ). Hence the trapezoidal rule of integration gives us a very simple formula. Usually this rule is not very accurate, but since we found that $\frac{\partial n(r, \mu, t)}{\partial \mu}$ is a slowly changing function of μ , we decided that the advantage of simplicity in this case outweighs the accuracy lost.

$$\int_{-1}^{+1} n(r, \mu, t + \Delta t) d\mu \approx \frac{1}{2} \Delta \mu [n(r, -1, t + \Delta t) + 2n(r, -1 + \Delta \mu, t + \Delta t) + \dots + 2n(r, 1 - \Delta \mu, t + \Delta t) + n(r, 1, t + \Delta t)]$$

In our next operation we sum $[n(r, -1, t + \Delta t) + 2n(r, -1 + \Delta \mu, t + \Delta t) + \dots + n(r, 1, t + \Delta t)]$ (For a discussion of the $(1/2)\Delta \mu$ term see the next section). This is performed on the tabulator, and at the same time a new small deck is summary punched.

Finally N , the total number of neutrons, is computed.

$$N(t + \Delta t) = \int \bar{n}(r, t + \Delta t) d(r^3) = 3 \int \bar{n}(r, t + \Delta t) r^2 dr \approx \sum \bar{n}(r, t) (3r^2 \Delta r)$$

$(3r^2 \Delta r)$ is independent of time. Hence we have a fixed deck containing r and $(3r^2 \Delta r)$. We merge this deck with the small deck and perform a group-multiplication, accumulating N in the summary counter.

This section was meant only as a brief outline of the method used. There are a number of problems that were not even touched upon, such as how to set the problem up, how to get $\bar{n}(t)$ and $\bar{n}(t + \Delta t)$ into the same deck, how to keep $\bar{n}(t - \Delta t)$, and how to handle the $1/2 \Delta \mu$ factor. These will be discussed in Section 7.3. In Section 7.4 we will give an outline of the eight operations. In Section 7.5 we will give the plugboard diagrams, and a description of the plugboards.

7.3 PROCEDURE FOR STARTING A PROBLEM

Let us assume that an actual problem is given. We shall still, for the sake of simplicity, restrict ourselves to the spherically symmetric case. We shall assume that σ and f are known at all points.

Our first problem is to choose the intervals Δr , $\Delta \mu$, and Δt . (For the actual problem it is not necessary to know v or Δt . We can use $v \Delta t$ instead of Δt , and α/v for α .) We want to choose $v \Delta t$ as large as possible in order to shorten our work. But we want it to take several cycles for the neutron to pass through the material. A reasonable value for $v \Delta t$ is about $1/50$ the radius of the material. Next we choose Δr . It is best to have the same Δr all through the material; but if that would require too many intervals and if there is some less important material near the outside, it may be better to choose a larger interval on the outside. Δr should be of the same order of magnitude as σ , but preferably smaller than σ . Once Δr is chosen we have a good check whether $v \Delta t$ is reasonable. $v \Delta t$ should be smaller than Δr , otherwise we get too little detail. One possible choice of these intervals is to let $\Delta r = 1/2 \sigma$ and $v \Delta t = 1/2 \Delta r$.

Our next problem, choosing $\Delta \mu$, is more difficult. We have to make sure that $|\delta \mu| \leq \Delta \mu$. ($|\delta r|$ is always $\leq \Delta r$, since Δr is at most $v \Delta t \leq r$.) For large r , $\delta \mu$ will be small; but if we have too many intervals, for small r , $\delta \mu$ can easily exceed $\Delta \mu$. We choose the smallest $\Delta \mu$ first. We chose this to be .25. ($\mu = -1, -.75, -.5, -.25, 0, .25, .5, .75, 1$) Then we com-

puted the $\delta\mu$'s. (Please note that the value of $\delta\mu$ does not depend upon the choice of $\Delta\mu$.) For small r we decided to use some of the same values of μ (though not all of them, to increase $\Delta\mu$). We also insisted on getting only one $\Delta\mu$ for each r . Therefore $\Delta\mu$ had to be a multiple of .25 and a factor of 2. This left us $\Delta\mu = .25, .5, 1, 2$, with 9, 5, 3, 2 values of μ , respectively. When $\Delta\mu = .25$ turned out to be too small, we tried .5, etc. It turned out that our two inside points had to have $\Delta\mu = 2$, the next one had $\Delta\mu = 1$, the next one $\Delta\mu = .5$ and all the others had $\Delta\mu = .25$. There are, of course, many other ways of choosing $\Delta\mu$; but this seems as reasonable as any.

Once we have $v\Delta t$, Δr , and $\Delta\mu$, we can compute the a_1 . This is a simple but laborious process.

$$a_1 = \frac{|\delta Y \delta \mu|}{\Delta Y \Delta \mu} e^{-\sigma v \Delta t}$$

$$a_2 = \frac{|\delta Y|(\Delta\mu - |\delta Y|)}{\Delta Y \Delta \mu} e^{-\sigma v \Delta t}$$

$$a_3 = \frac{(\Delta Y - |\delta Y|)|\delta \mu|}{\Delta Y \Delta \mu} e^{-\sigma v \Delta t}$$

$$a_4 = \frac{(\Delta Y - |\delta Y|)(\Delta\mu - |\delta \mu|)}{\Delta Y \Delta \mu} e^{-\sigma v \Delta t}$$

$$a_5 = \frac{1+f}{2} \left\{ 1 - \frac{1}{\sigma v \Delta t} + \frac{e^{-\sigma v \Delta t}}{\sigma v \Delta t} - \frac{|\delta Y|}{\Delta Y} \frac{1}{\sigma v \Delta t} + \frac{|\delta Y|}{\Delta Y} \left[\frac{2(1 - e^{-\sigma v \Delta t})}{(\sigma v \Delta t)^2} - \frac{e^{-\sigma v \Delta t}}{\sigma v \Delta t} \right] \right\}$$

$$a_6 = \frac{1+f}{2} \frac{|\delta Y|}{\Delta Y} \left[\frac{1 + e^{-\sigma v \Delta t}}{\sigma v \Delta t} - \frac{2(1 - e^{-\sigma v \Delta t})}{(\sigma v \Delta t)^2} \right]$$

$$a_7 = \frac{1+f}{2} \left\{ -e^{-\sigma v \Delta t} + \frac{1 - e^{-\sigma v \Delta t}}{\sigma v \Delta t} - \frac{|\delta Y|}{\Delta Y} \left[\frac{2(1 - e^{-\sigma v \Delta t})}{(\sigma v \Delta t)^2} - \frac{2e^{-\sigma v \Delta t}}{\sigma v \Delta t} - e^{-\sigma v \Delta t} \right] \right\}$$

$$a_8 = \frac{1+f}{2} \frac{|\delta Y|}{\Delta Y} \left[\frac{2(1 - e^{-\sigma v \Delta t})}{(\sigma v \Delta t)^2} - \frac{2e^{-\sigma v \Delta t}}{\sigma v \Delta t} - e^{-\sigma v \Delta t} \right]$$

With the aid of these formulae we can compute all the $a_1(r', \mu')$. Then we want to know what r, μ equal for each $a_1(r', \mu')$.

$$a_1: Y = Y' \pm \Delta Y, \mu = \mu' \pm \Delta \mu$$

$$a_2: Y = Y' \pm \Delta Y, \mu = \mu'$$

$$a_3: Y = Y', \mu = \mu' \pm \Delta \mu'$$

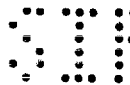
$$a_4: Y = Y', \mu = \mu'$$

$$a_5: Y = Y'$$

$$a_6: Y = Y' \pm \Delta Y$$

$$a_7: r = r'$$

$$a_8: r = r' \pm \Delta Y$$



The + sign is to be used for $\Delta r(\Delta \mu)$ when $\delta r(\delta \mu)$ is negative. Otherwise the minus sign is used.

We are now ready to prepare the masterdecks. We punch i in column 1, r in columns 2-3, μ in 4, a_i in 5-11, the problem no. in 19, r' in 58-59, and μ' in 70. (To these decks we shall add dummy-cards later.) It is advisable to keep several copies of the masterdecks on hand. Since we have to use a new masterdeck on every cycle, it is also useful to change the card layout frequently. By moving the product into a new field (changing the punching on op. 4, and reading in op. 6), we can use the masterdecks several times.

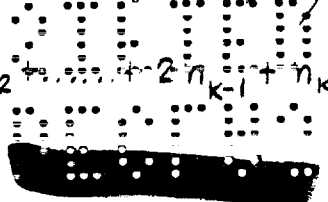
In punching t, r, and μ we replaced the real values by a key. We set Δt equal to 1. We called the center 1, the next point 2, etc. We also replaced $\mu = -1$ by 0, $\mu = -.75$ by 1, etc. Whenever a reference is made to t, r, or μ "on the card", we mean the symbol, not the real value.

Next we choose two distributions: $n(r, \mu, 0)$ and $n(r, \mu, 1)$. These can be chosen arbitrarily, because the initial distribution does not effect the asymptotic solution. However, through sufficient practice we can choose curves that will shorten our work considerably. Our own starting data was not very good from this point of view. The best we can say is that n is a monotone increasing function of μ , and it is a rapidly decreasing function of r. These two sets of curves should be punched on cards according to the layout. Then these two decks are put through operation 7 to get the corresponding small decks.

We also prepare a fixed deck according to the layout.

We are still left with the three problems mentioned at the end of the last section. One of them is caused by the $1/2 \Delta \mu$ factor in the formula

$$\bar{n} = \frac{1}{2} \Delta \mu (n_1 + 2n_2 + \dots + 2n_{k-1} + n_k)$$



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The easiest way of handling this is to replace $\bar{n}(r', \mu', t)$ by $\frac{1}{2} \Delta \mu' n(r', \mu', t)$; to replace $a_i (i=1, \dots, 4)$ by $\frac{\Delta \mu'}{\Delta \mu} a_i$ ($\frac{\Delta \mu'}{\Delta \mu} = 1$ except near the center where $\Delta \mu$ changes); and to replace $a_i (i=5, \dots, 8)$ by $\frac{1}{2} \Delta \mu' a_i$. We then get in operation 6:

$$\frac{1}{2} \Delta \mu' n(r', \mu', t + \Delta t) = \sum_{i=1}^4 \left(\frac{\Delta \mu'}{\Delta \mu} \right) a_i \left(\frac{1}{2} \Delta \mu' n_i \right) + \sum_{i=5}^8 \left(\frac{1}{2} \Delta \mu' a_i \right) \bar{n}_i = \frac{1}{2} \Delta \mu' \left[\sum_{i=1}^4 a_i n_i + \sum_{i=5}^8 a_i \bar{n}_i \right]$$

which is correct. In operation 7 we get:

$$\bar{n} = \left(\frac{1}{2} \Delta \mu' n_1 \right) + 2 \left(\frac{1}{2} \Delta \mu' n_2 \right) + \dots + \left(\frac{1}{2} \Delta \mu' n_k \right)$$

which is also correct. But we must remember that our listings show $\frac{1}{2} \Delta \mu' n_k$ instead of n .

Next we face the problem of having to add both $a_i \bar{n}(t)$ and $a_i \bar{n}(t + \Delta t)$ terms in the same n . We found the following to be a fruitful approach. In cycle $t - \Delta t$ we compute all the $a_i \bar{n}(t)$, but we save the $a_7 \bar{n}(t)$ and $a_8 \bar{n}(t)$ until the next cycle. In their place we use the cards saved from the last cycle. Then at cycle t the two sets of $a_i \bar{n}(t)$ will be available from the last cycle, the two $a_i \bar{n}(t + \Delta t)$ are computed during the cycle. Thus $a_7 \bar{n}(0)$ and $a_8 \bar{n}(0)$ have to be done before the problem is started. Then in cycle one we proceed normally until operation 5. In operation 5 we sort on column 1 to separate the a_i on i . Here we replace the decks $i=7, 8$ and replace them by $a_7 \bar{n}(0)$ and $a_8 \bar{n}(0)$. The two decks removed will be used in a similar manner in cycle 2.

It turns out that the same trick will solve the problem of keeping $\bar{n}(t - \Delta t)$. We have $\bar{n}(t)$ on the small deck. (This was computed in operation 7 of the last cycle.) What we need is $\bar{n}(t)$ of the last cycle. Therefore we put some dummy a_7 cards into the masterdecks, one for each r . These have $a_7 = 1$. Let us say that we are running cycle t . $\bar{n}(t + \Delta t)$ will multiply this $a_7 = 1$, and the product card (together with all a_7, a_8) will be removed and saved for the next cycle. In operation 6 of $t + \Delta t$ we transfer this "product" onto an n card, and in operation 7 to the proper \bar{n} card. This card will be used in

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cycle $t+2\Delta t$ and will have $\bar{n}(t+\Delta t)$ on it as described. This solves the problem. These dummy cards must have an "X" in 79 to stop the tabulator from adding them up with the regular products.

A very useful trick is to change the "i" which refers to problem no.1. It is best to change it to 9. For example, if we are running problem 1, replace the a_1 by a_9 . This enables us to separate the masterdecks from the small and large decks in operation 5, and at the same time to sort the a_i on i. This also ensures that the a_8 will not be the last a_i in any of the groups of eight cards; this is necessary for plugboard 6 to function correctly.

7.4 OUTLINE OF THE OPERATIONS

Operation 1. Purpose: to compute $\bar{n}^2(t)$.

Procedure: We take the small deck and put it through the multiplier with plugboard 1.

Operation 2. Purpose: To divide $\bar{n}^2(t)$ by $\bar{n}(t-\Delta t)$, i.e., to compute $\bar{n}(t+\Delta t)$ approximately.

Procedure: We put the small deck through the multiplier with plugboard 2. Be sure not to use a blank leadcard. (On a blank card 0:0 causes trouble.)

Operation 3. Purpose: To merge deck for the main multiplication.

Procedure: Sort masterdecks on column 1. Separate a_1-a_4 from a_5-a_8 . Merge large deck with a_1-a_4 on columns 2-4 (be sure large deck precedes masterdeck.) Merge small deck with a_5-a_8 on columns 2-3. (Be sure small deck precedes masterdeck.)

Operation 4. Purpose: To compute the products.

Procedure: Put the merged decks through the multipliers, using plugboard 4, and using a leadcard with an "X" in 30.

Operation 5. Purpose: To separate masterdecks from large and small decks. To replace $a_7\bar{n}(t+\Delta t)$ and $a_8\bar{n}(t+\Delta t)$ by $a_7\bar{n}(t)$ and $a_8\bar{n}(t)$. To sort the masterdecks for fabrication.

Procedure: Sort on cols. 1-6. Remove the small and large decks from pocket 1 (or whatever the problem no. is) and replace the cards in pockets 7 and 8 by the cards saved from the last cycle. Sort on cols. 68-70. (See the last paragraph of section 7.3.)

Operation 6. Purpose: To compute $n(t + \Delta t)$. To transfer $\bar{n}(t)$. To transfer all permanent information.

Procedure: Put the masterdecks through tabulator using plugboard 6 in the tabulator, and 6-S in the summary punch. Use a leadcard with $t + \Delta t$ in cols. 1-2, and an "X" in 40.

Operation 7. Purpose: To compute $\bar{n}(t + \Delta t)$. To transfer $\bar{n}(t)$. To transfer all permanent information.

Procedure: Put the new large deck through the tabulator using plugboard 7 in the tabulator, and 7-S in the summary punch. Use a runout card with an "X" in 17.

Operation 8. Purpose: To compute $N(t + \Delta t)$.

Procedure: Merge the fixed deck with the new small deck on cols. 1-2. (The fixed deck precedes the small deck.) Put the merged deck through a multiplier using plugboard 8. Use a lead card with an "X" in 80. $N(t + \Delta t)$ is accumulated in the summary counter. (Be sure to clear summary counter before starting operation.)

After operation 8 $\left(\frac{\alpha}{V}\right)$ can be computed locally.

$N(t)$ is assumed to tend to $e^{\alpha t} n(\gamma, \mu)$

$$\frac{N(t + \Delta t)}{N(t)} = \frac{e^{\alpha(t + \Delta t)} n(\gamma, \mu)}{e^{\alpha t} n(\gamma, \mu)} = e^{\alpha \Delta t} = e^{\left(\frac{\alpha}{V}\right) V \Delta t}$$

$$\log \left[\frac{N(t + \Delta t)}{N(t)} \right] = (V \Delta t) \left(\frac{\alpha}{V}\right)$$

$$\therefore \frac{\alpha}{V} = \frac{1}{V \Delta t} \left[\log N(t + \Delta t) - \log N(t) \right]$$

7.5 DESCRIPTION OF THE PLUGBOARDS, AND PLUGBOARD DIAGRAMS

X-1. The purpose of this operation is to compute $\bar{n}^2(t)$ on the small deck. The plugboard is an ordinary multiplier board on which $\bar{n}(t)$, cols. 11-15, is used both as multiplier and multiplicand. The product

is punched in cols. 21-28. (Figure 1)

X-2. This plugboard is wired for a simple division. The dividend is taken from 21-28, the divisor from 16-20. The quotient is computed to as many digits as possible, and the answer is punched in cols. 31-36. Note: In both the foregoing plugboards it is assumed that the first digit of \bar{n} is not greater than a 3. If this is not the case, an extra place must be allowed on the left in the product in X-1, and in the dividend in X-2. (Figure 2)

X-4. We now have the small and large decks merged with their respective masterdecks. The quantities in 31-36 are used as group multipliers. The group multiplication is under the control of an "X" in 30. Cols. 5-11 in the masterdecks, the a_i , are used as multiplicands. The products are punched in cols. 12-18. (Figure 3)

X-6,
X-6-3. The products have been computed, and we now want to add up the eight terms of each $n(r', \mu', t + \Delta t)$. The masterdecks are sorted on r' and μ' . Thus the eight terms adding into a particular n follow each other. We use a leadcard with an "X" in 40, and $t + \Delta t$ in 1-3. This number is read into counter 2B and is kept there till the end of the operation. The cycle number $t + \Delta t$ is punched on every card by the summary punch, and it is printed at the end of the listing. On the following cards the products are added into counters 8A and 8B. On a change in μ (end of the 8-card group) a total is taken on 8A and the n is both listed and summary punched. 8B computes the total of all n . The problem no., r , and μ have to be read from one of the eight cards. For this we use digit selector #1. When an 8 is picked up in col. 1 (1 of a_i), selector D is turned on. So the permanent data is read from the card following a_8 . (This is why a_8 should not be the last of the 8 cards.) This information is listed and summary punched. (Figures 4 and 5)

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Figure 1

Plugboard Diagram

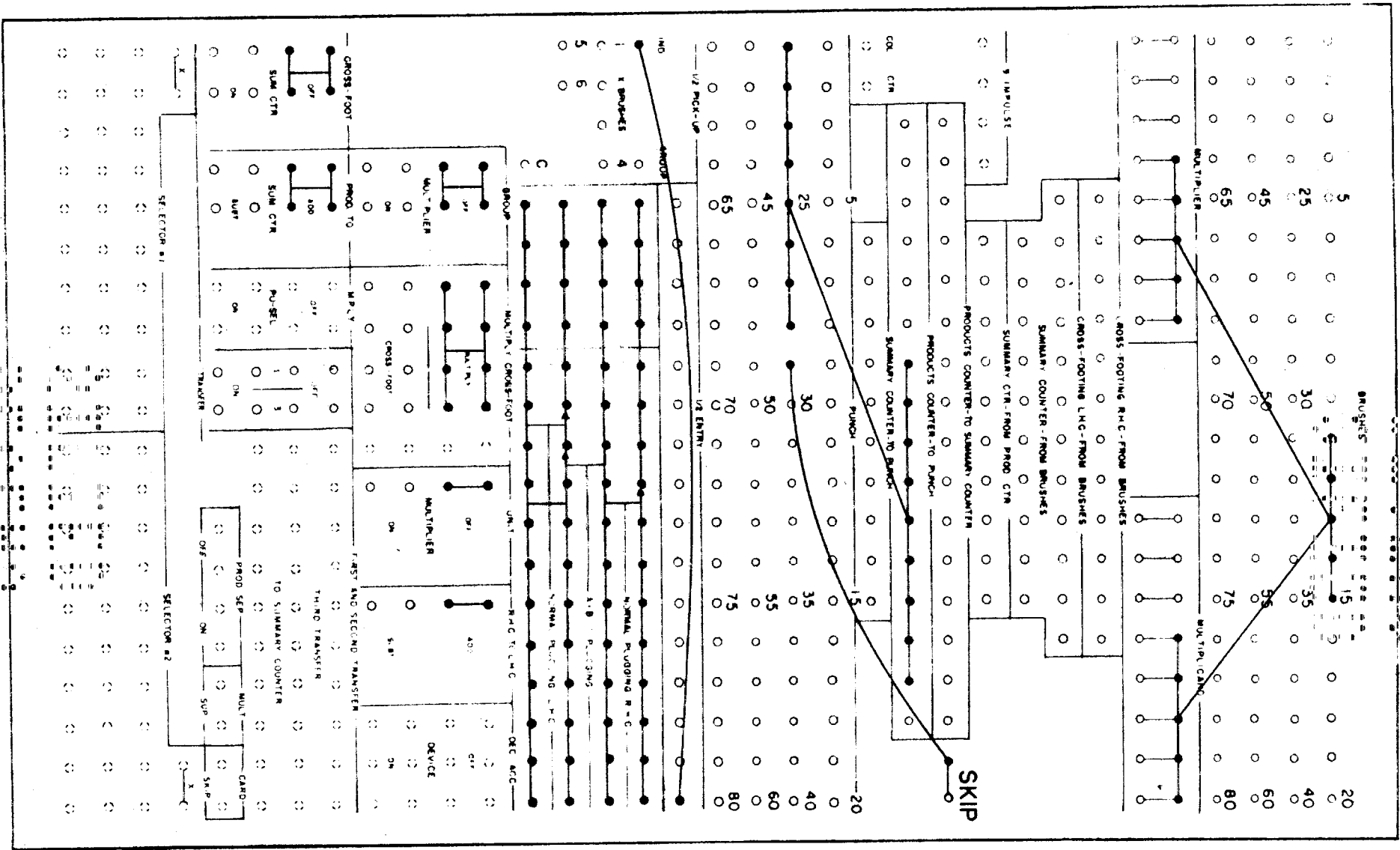
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INTERNATIONAL BUSINESS MACHINES CORPORATION

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6-4042

FORM 32 7080 5 END
11-14-50-1-15



CUSTOMER _____

DEPT. _____

TITLE OF REPORT _____

DATE _____

ELECTROTYPE NUMBERS OF CARDS INVOLVED: _____

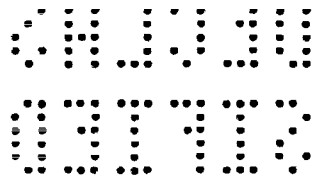
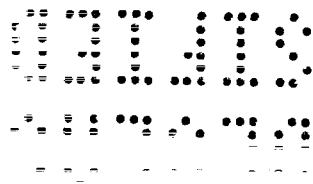
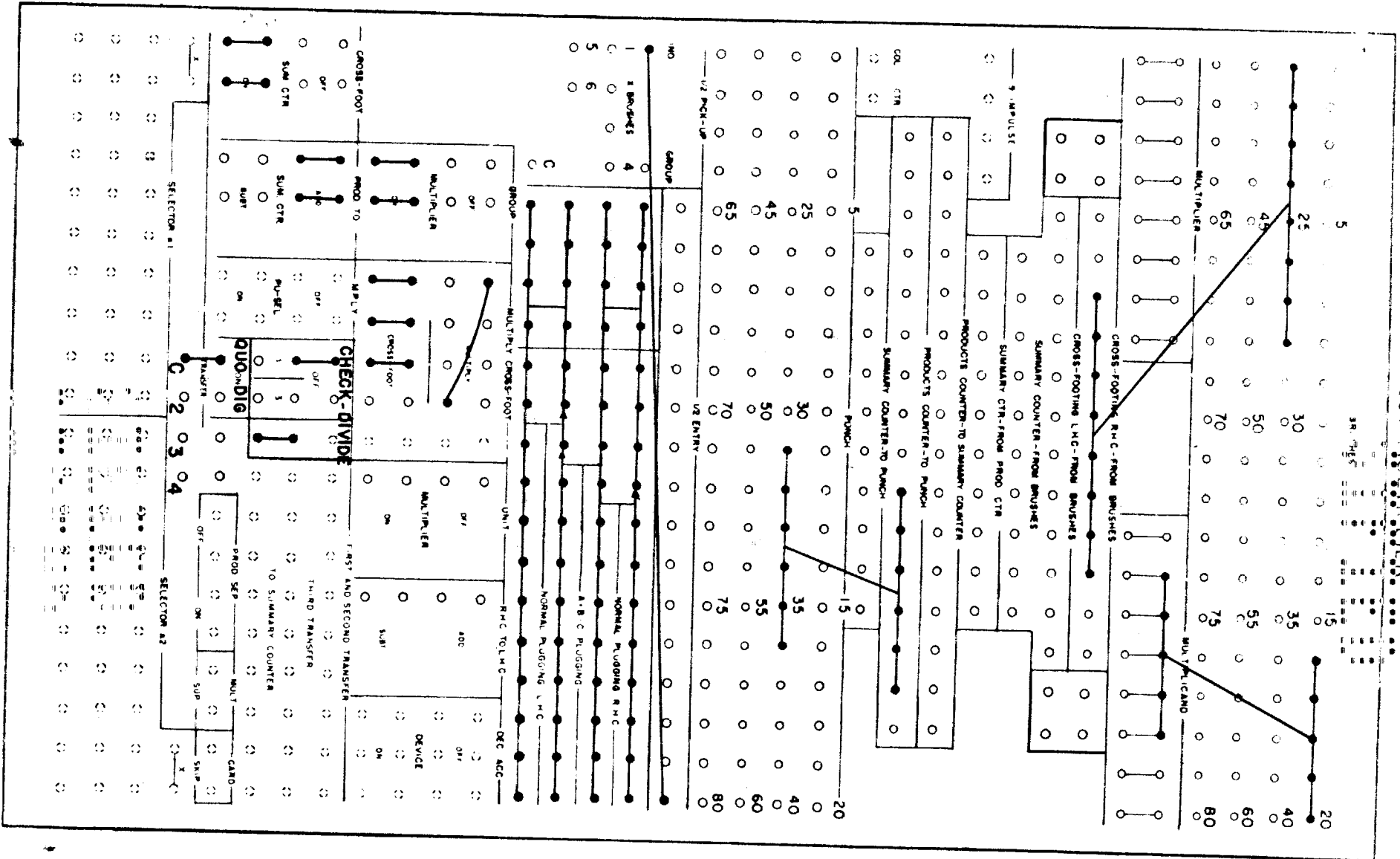


Figure 2
Plugboard Diagram



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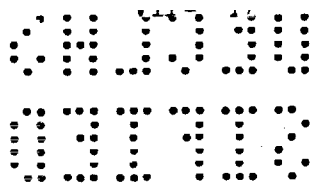
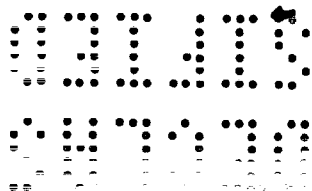


Figure 3

Plugboard Diagram

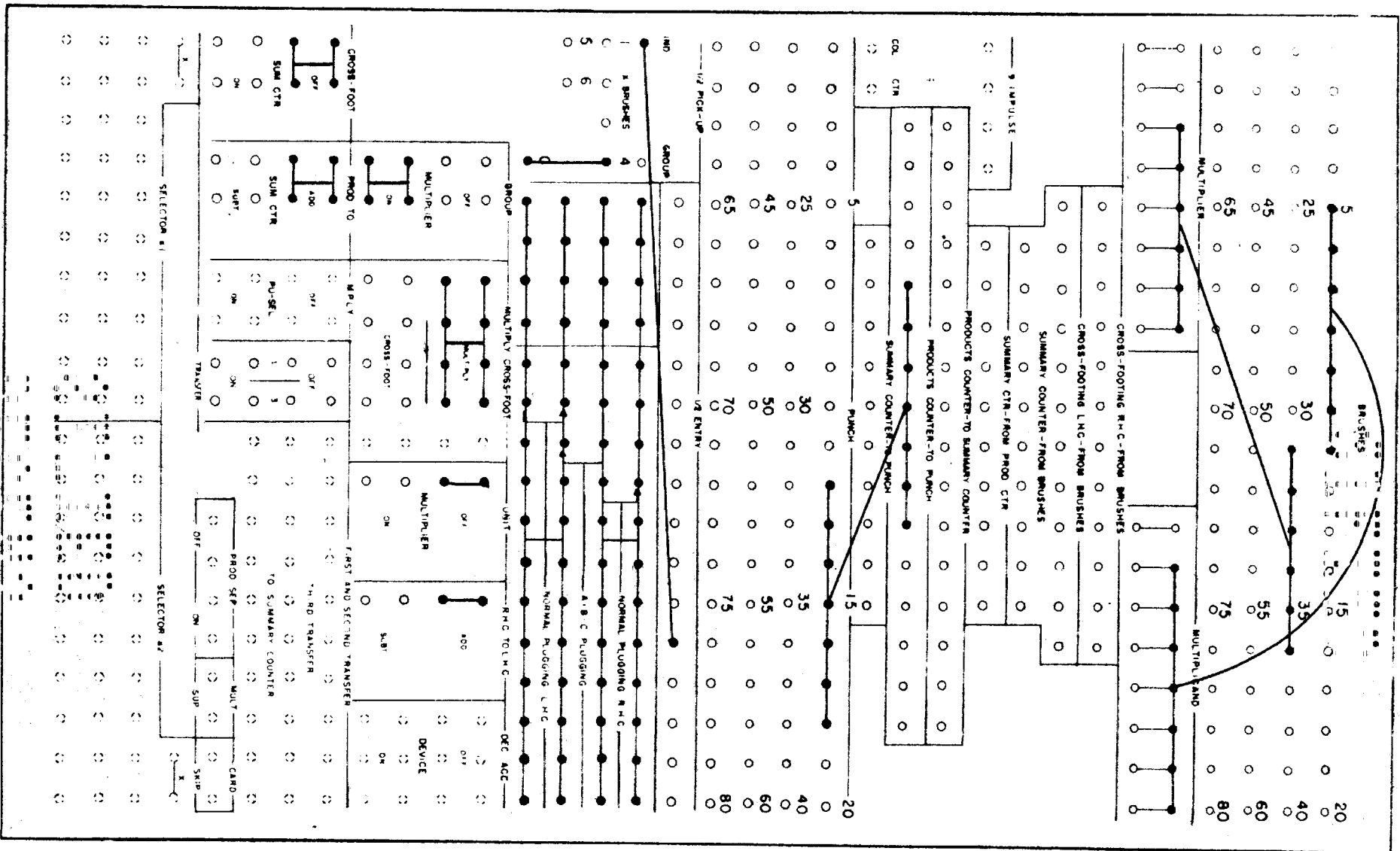


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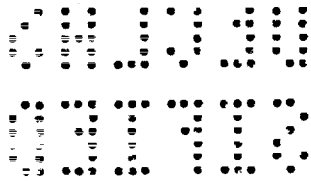
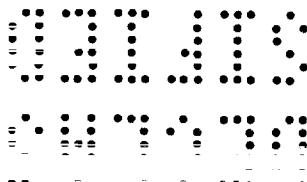
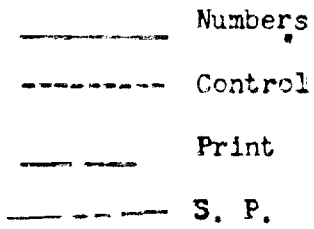


Figure 4

Plugboard Diagram



011434
03110

Figure 5
Plugboard Diagram

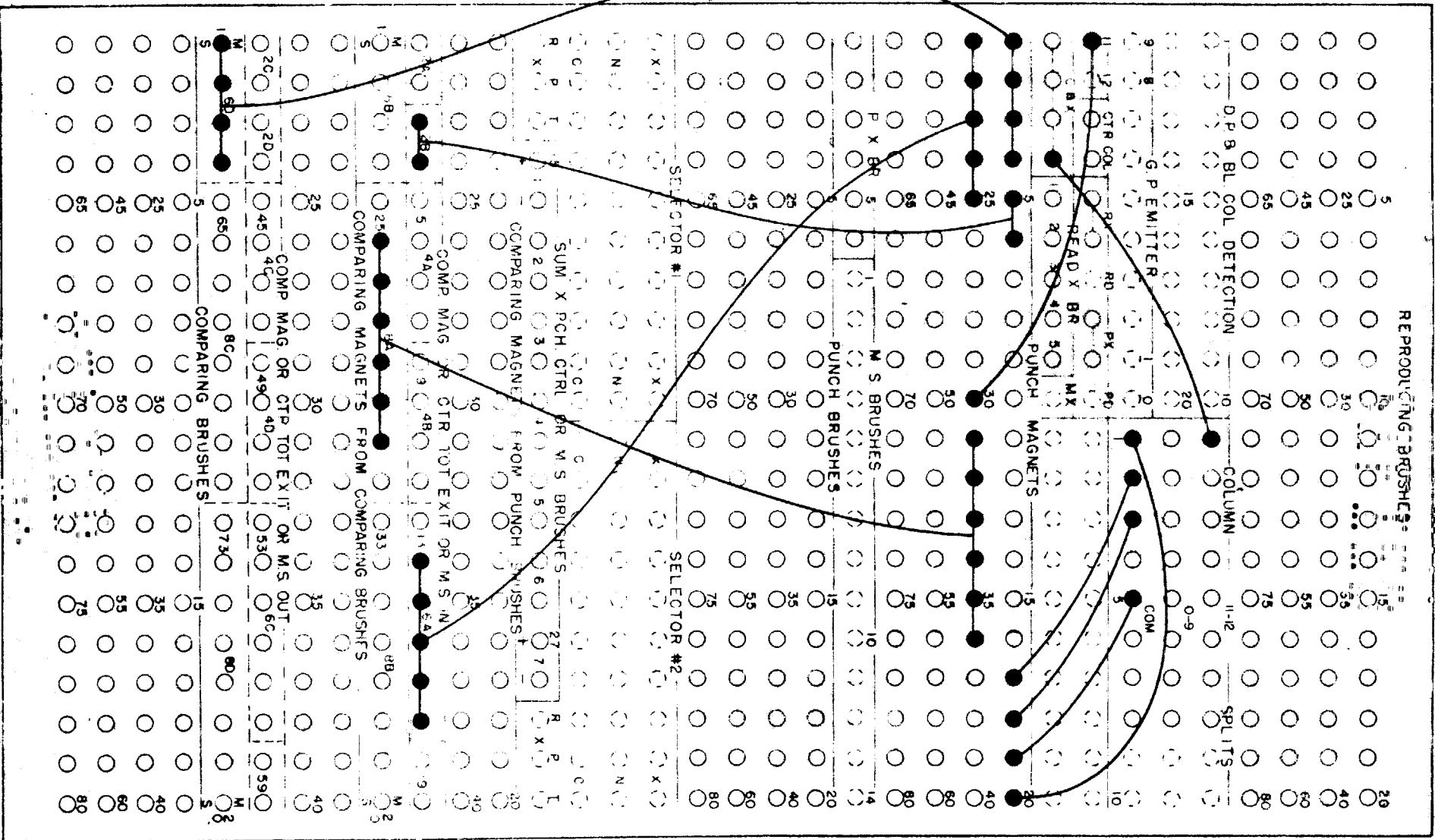
011434
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INTERNATIONAL BUSINESS MACHINES CORPORATION
TYPE 513 AUTOMATIC REPRODUCING PUNCH PLUGBOARD
FOR SUMMARY PUNCHING - ALPHABETIC ACCOUNTING MACHINE

FORM 32 9188-3 END
1200 PERG-4-54

ELECTROTYPE NUMBERS
OF CARDS INVOLVED:



TITLE OF REPORT _____

DATE _____

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DEPT. _____

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$\bar{n}(t)$ is taken from the summary cards and read into counter 6A when selector C is activated by the "X" in 79. $\bar{n}(t)$ is listed and summary punched. An "X" is gangpunched in cols. 20 and 30 on every card. The last remaining problem is the summary punching of the "X" in 17, 18, or 19. By reading a cardcount impulse negatively into 8D we assure ourselves that 8D will have a negative sum. We put the counter on balance conversion and use the summary X-punch control for summary punching. Digit selector #2 activates selector F on a 0 in col. 1, and selector E on an 8. If μ equals 0, the "X" is punched in 17. If $\mu \neq 0$, the impulse is carried into selector E. If $\mu = 8$, the "X" is punched in col. 19, otherwise it is punched in 18. The listing of these "X"'s is done similarly by the use of the total symbols. It is a good check to watch the listings in numerical typewriters 3-5. An * in 3 should be followed by several CR in 4 and by an * in 5, etc.

There is a set of wires that is no longer necessary under our revised method. They are, however, included because they illustrate a very interesting method. Under our new method all the a_i are positive, and digit selectors 2,3 as well as selectors 1-3 should not be connected; instead a plug to "0" impulse should be connected to "+" of the counters 8A, 8B. In our original method we used an extrapolation formula in case of negative $\delta r, \delta \mu$. Therefore, 8A had to subtract on about half our cards. The use of an "X" for a minus sign is very cumbersome because of the large number of cards, and we felt it safer to use a different method. We noticed that most of our minus signs occurred on certain combinations of i and μ . Therefore, $i = 2, 6, 8$, or 9 and $\mu = 0, 1, 2, 3$, or 4 will act as a minus sign. There are a few additional negative a_i , and therefore an "X" in 39 will also make the counters subtract. If none of the

VII-21

20 combinations occurs, and there is no "X" in 39, the counters add.

X-7
X-7-S

The main purpose of this operation is to perform the trapezoidal integration on n . The coefficients of this integration are 1, 2, 2, ..., 2, 1. Therefore, the cards with "X" in 17, 19 are added once, the others are added twice. This is done completely under the control of the different "X"'s. Let us suppose that we have only three values of μ , so that we have three cards with "X"'s in 17, 18, 19 respectively. On each card n is read into selector B. On the first card this selector is on, hence n is read into 8A. On the next card n is added into 8B (through selectors B, C), and into 8C, 8D (through selector D). On the last card the n is added into counters 8C, 8D only (through selectors B, C). Now we have all the necessary n 's in counter 8A, 8B, 8C (8D), and they are summed by total-cycle-transfers. On the last card 8A transfers to 8B, and on the first card of the next group (after the next n has been read into the counter 8A) 8B transfers to 8C and 8D. Then a total is taken giving us \bar{n} in 8C. The difficulty in this procedure comes up on taking a total. We take a total on the first card of the next group, and therefore 8A clears at the wrong time. We avoided this by not taking a total on 8A; instead we clear it when it transfers its information. (This is done by the 6 wires from counter total exit to counter list exit.) In order to complete the last group, we must use a runout card with an "X" in 17. (Figures 6 and 7).

The $\bar{n}(t)$ is read into counter 6B, from which it is listed and summary punched. For simplicity's sake the problem number is just listed and gangpunched (not summary punched). r and t are read into counters 2C and 2D. But since we want r for only one μ , we must send it through selector A, which is turned on by the first μ in each group only.

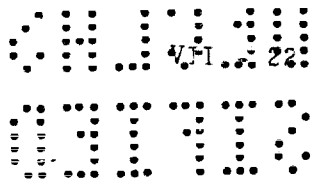
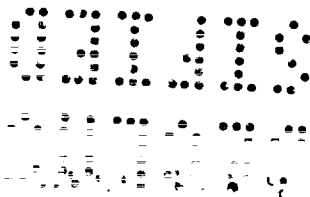


Figure 6

Charge explanation as follows:

- — — — — Numbers
- — — — — Control
- — — — — Print



01100
01110

Figure 7
Plugboard Diagram

01110
01100

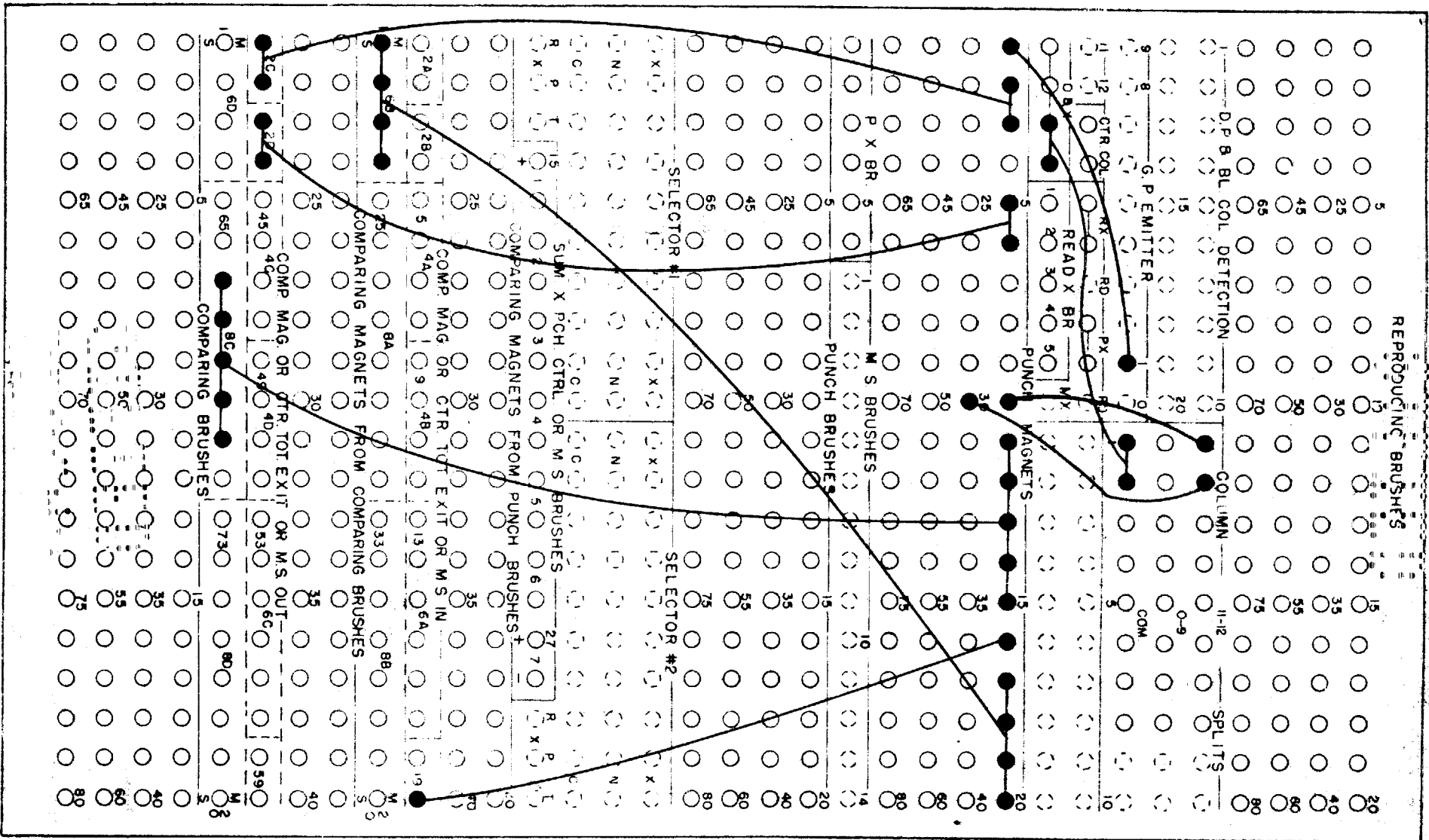
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VII-2

X-3. $(3r^2 \Delta r)$ is used as a group multiplier to multiply $\bar{n}(r, t + \Delta t)$. The products are added up in the summary counter. The cards are skipped out without punching. Use a leadcard with an "X" in 80. (This "X" controls the group multiplication.) $\bar{n}(t + \Delta t)$ is shown in the summary counter at the end of the operation. Be sure to clear summary counter before starting the operation. (Figure 8).

CARD-LAYOUTS

LARGE DECK	SMALL DECK	MASTERDECKS	FIXED DECK
column item	column item	column item	column item
1 Problem no.	1 Problem no.	1 1 of a_1	1 Problem no.
2-3 r	2-3 r	2-3 r	2-3 r
4 μ	5-6 t	5-11 a_1	4-9 $3r^2 \Delta r$
5-6 t	11-15 $\bar{n}(t - \Delta t)$	12-18 product	X 20 group multiplier
21-25 $\bar{n}(t - \Delta t)$	16-20 $\bar{n}(t)$	19 Problem no.	
31-36 $n(t)$	21-28 $\bar{n}^2(t)$	68-69 r'	
X 17 $\mu = -1$	31-36 $\bar{n}(t + \Delta t)$	70 μ'	
X 18 $\mu \neq \pm 1$	X 10 denotes small deck	X 39 negative a_1^*	
X 19 $\mu = +1$	X 30 group multiplier	X 79 dummy card	
X 30 denotes large deck			
X 30 group multiplier			

*Under revised system there are no negative a_1 .

VII-2

41138
031712

Figure 8
Plugboard Diagram

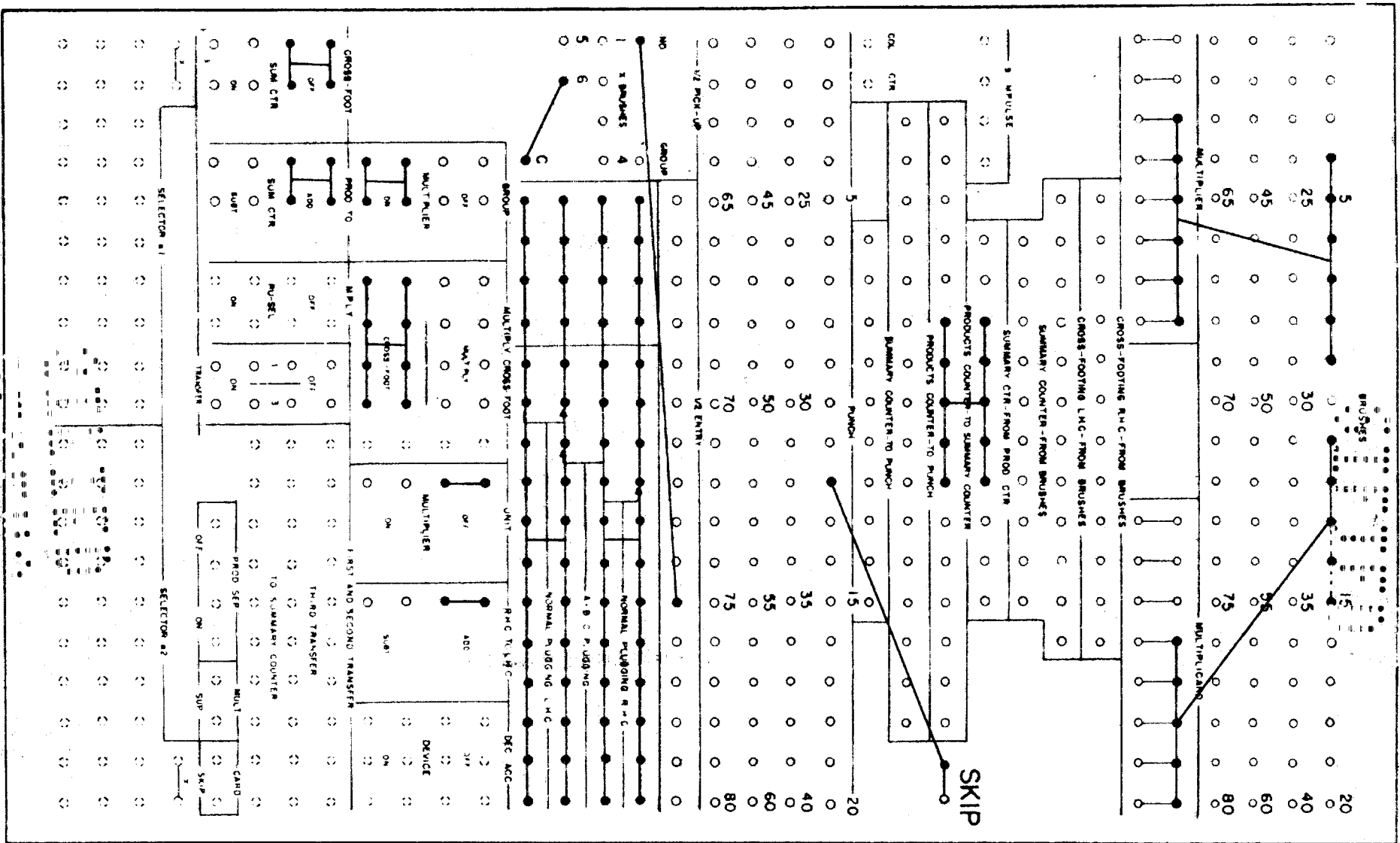
01110
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INTERNATIONAL BUSINESS MACHINES CORPORATION

TYPE 601 MULTIPLIER

6-4042

FORM 32-1090 SEND
MAY 1962



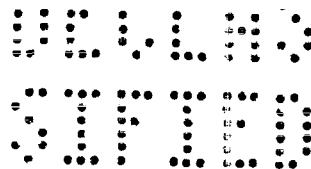
CUSTOMER _____

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ELECTROTYPE NUMBERS OF CARDS INVOLVED:



CHAPTER 8

MISCELLANEOUS PROBLEMS IN NUMERICAL CALCULATION

D. Flanders and P. Whitman

8.1 SOLUTION OF EQUATIONS (Flanders)8.1-1 Introduction; Quadratic Formula

A common problem in numerical computations is: find the solution or solutions of a given equation. In certain cases this can be done by an explicit formula, but in many cases it must be done by approximation or by a succession of approximations.

An equation which can be solved explicitly is the general quadratic equation

$$ax^2 + bx + c = 0 \quad (1)$$

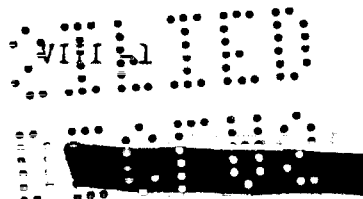
where a, b, and c are given. Its solutions are

$$x = \frac{-b + \sqrt{b^2 - 4ac}}{2a} \quad \text{and} \quad x = \frac{-b - \sqrt{b^2 - 4ac}}{2a} \quad (2)$$

usually called the "quadratic formula". An equation such as $ax^4 + bx^2 + c = 0$ can be reduced to the form (1) by the substitution $z = x^2$. For equations of the types

$$ax^3 + bx^2 + cx + d = 0$$

$$\text{and} \quad ax^4 + bx^3 + cx^2 + dx + e = 0$$



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there are also explicit solutions⁽¹⁾, but in practice it is easier to apply

(1)

L. E. Dickson, First Course in the Theory of Equations, New York (1922) pp. 45-54.

J. B. Rosenbach and E. A. Whitman, College Algebra, revised edition, Boston (1939) pp. 265-271.

F. R. Rider, College Algebra, New York (1940) pp. 203-208 (or almost any other book on this subject).

a method (such as Newton's method, about to be described) which is applicable to equations generally.

8.1-2 Removing Known Solutions

However, after all but two of the solutions x_1, x_2, \dots, x_n of

$$a_0 x^n + a_1 x^{n-1} + \dots + a_n = 0 \tag{3}$$

have been found, the remaining two can be found by dividing out the factors $(x - x_1)$ corresponding to the known roots. For this purpose, however, it is advisable to find the "known" roots to one or two more figures than desired, to allow for rounding-off errors, etc., in the division.

The division is most conveniently done by "synthetic division"⁽²⁾.

(2)

Rosenbach and Whitman, loc. cit., pp. 229-230.

Rider, loc. cit., pp. 176-177.

For example,

$$1.337 x^4 + 68.927 x^3 + 1082.456 x^2 + 5115.498 x - 3333.796 = 0 \tag{4}$$

has the solutions $x_1 = 0.578303$ and $x_2 = -26.8019$ (see below, Section 8.1-3).

Divide these out successively:

$$1.337 + 68.927 + 1082.456 + 5115.498 - 3333.796 \quad \boxed{.578303} \tag{5}$$

$$.7732 \quad 40.3078 + 649.2977 - 3333.799 \tag{6}$$

0.578303

$$1.337 + 69.7002 + 1122.7638 + 5764.7957 = 0 \quad | \quad -26.8019 \quad (7)$$

$$- 35.83414 - 907.67475 + 5764.7952 \quad (8)$$

$$1.337 + 33.86606 + 215.08905 = 0 \quad (9)$$

Here line (7) represents simultaneously the quotient from the first division and the dividend for the second division. That the remainder comes out zero in lines (7) and (9), to within an amount which can be accounted for by significant figures⁽³⁾ and rounding-off errors, shows that 0.578303 and -26.8019

(3)

As discussed in Section 8.4-1, we have sometimes carried more figures in the computation than are, strictly speaking, significant.

are indeed solutions of (4), while the remaining two roots must by (9) be solutions of

$$1.337 x^2 + 33.86606 x + 215.08905 = 0, \quad (10)$$

and so can be found by the quadratic formula (2); they turn out to be complex numbers.

8.1-3 Method of Successive Interpolation

One method⁽⁴⁾ of finding the solutions of an equation - the equation need

(4)

Scarborough, loc. cit., pp. 174-178.

Whittaker and Robinson, loc. cit. pp. 92-93.

not be of the type (3) - is sometimes called the "method of false position", but might more appropriately be called the method of successive interpolation. Suppose the equation to be solved is

$$f(x) = 0 \quad (5) \quad (11)$$

(5)

An equation $g(x) = h(x)$ can be written in the form (11) by transposition.

First one must get a rough idea of the location of the solutions. If

0.578303

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nothing is known a priori, one may compute $f(x)$ for several values of x (for instance, $x = 0, \pm 1, \pm 2, \text{etc.}$) and observe that if $f(b)$ and $f(c)$ have opposite signs then there is a solution between b and c , provided $f(x)$ is continuous in this interval. Trouble may be encountered in case there are two solutions between a pair of successive integers, but the trend of the values of $f(x)$ will generally indicate what is happening here, and one may graph the function or take some non-integral values of x to separate the roots. Then, too, this method locates only real roots, but in numerical work we are usually (but not always) interested only in real numbers. With the known values $f(b)$ and $f(c)$ we may interpolate to find what value of x will give $f(x) = 0$; actually, of course, this is inverse interpolation (Section 2.1-4), but since we use linear interpolation (Equation (7)) no distinction between direct and inverse interpolation need be made. Let us denote by a_1 the interpolated value of x . Then compute $f(a_1)$. If interpolation were exact, then $f(a_1) = 0$; but since we used an approximation (linear interpolation) it can only be expected that $f(a_1)$ will be near zero. Then using either $f(b)$ or $f(c)$ - usually, whichever is smaller in absolute value - and $f(a_1)$ we may perform a similar interpolation or extrapolation to get a new approximate solution, a_2 . Then interpolating between $f(a_1)$ and $f(a_2)$ we get a_3 , and so on. Once well started, the process converges rapidly except for functions whose graphs have sharp bends near the points in question.

The process should be continued until two successive a_i have the same value to the desired accuracy.

The first approximation a_1 may, if desired, be obtained by graphing the calculated points (e.g. $x = 0, \pm 1, \pm 2, \text{etc.}$) and reading off the value of x for $f(x) = 0$, rather than by interpolation as indicated above. This method is useful when it is suspected that the curve has a sharp bend in the vicinity.

For convenience we may write the formula for linear interpolation in the

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special form used here:

DIFFERENTIAL

$$\left. \begin{aligned} a_{n+1} &= a_n + \Delta a_n \\ \Delta a &= - f(a_n) \frac{a_n - a_{n-1}}{f(a_n) - f(a_{n-1})} \end{aligned} \right\} \quad (12)$$

where, for starting, we may denote b by a_{-1} and c by a_0 (or vice versa).

8.1-4 Method of Iteration

A slight variation of the previous method is applicable if the given equation can be written in the form $x = f(x)$. Then once a first approximation a_1 to the solution has been obtained, say as in Section 8.1-3, then successive approximations can be obtained by $a_2 = f(a_1)$, $a_3 = f(a_2)$, etc. This process converges⁽⁶⁾ if $|f'(x)| < 1$ for x near the solution.

(6) Scarborough, loc. cit., p. 187.

8.1-5 Newton's Method

Another method, known as Newton's method⁽⁷⁾, applies to any equation,

$$f(x) = 0, \quad (13)$$

Provided that $f'(x)$ can be found and is not zero at or near a solution $x = r$.

(7) Scarborough, loc. cit., p. 178 ff.
 Whittaker and Robinson, loc. cit., p. 84 ff.
 Granville, Smith, and Longley, loc. cit., pp. 131-132.

If a_i is an approximation to a solution of (13), then as the next approximation we have

$$a_{i+1} = a_i - \frac{f(a_i)}{f'(a_i)} \quad (14)$$

or

$$\left\{ \begin{aligned} a_{i+1} &= a_i + \Delta a_i \\ \Delta a_i &= - \frac{f(a_i)}{f'(a_i)} \end{aligned} \right. \quad (15)$$

DIFFERENTIAL

SECRET

Once a reasonably accurate first approximation has been found (for instance by the same method as in Section 8.1-3) this process generally gives quite rapid convergence. The approximate error of a_{i+1} is given⁽⁸⁾ by

(8) Scarborough, loc. cit., pp. 182-183.

$$E_{i+1} \leq \frac{(\Delta a_i)^2}{2 |f'(a_i)|} \max_{a_i \leq x \leq a_{i+1}} |f''(x)| \quad (16)$$

In practice, however, one simply continues making new approximations by (14) or (15) until two successive a_i agree to the accuracy desired.

For example, as in Section 8.1-3, it is found that

$$1.337 x^4 + 68.927 x^3 + 1082.456 x^2 + 5115.498 x - 3333.796 = 0 \quad (17)$$

has a solution approximately equal to 0.57. Using (15) we have

$$f(x) = 1.337 x^4 + 68.927 x^3 + 1082.456 x^2 + 5115.498 x - 3333.796$$

$$f'(x) = 5.348 x^3 + 206.781 x^2 + 2164.912 x + 5115.498$$

Trial	1	2	3
a	0.570000	0.578315	0.578303
a ²	0.324900	0.334448	0.334434
a ³	0.185193	0.193416	0.193404
a ⁴	0.105560	0.111855	0.111846
f(a)	-53.366	0.080	0.002
f'(a)	6418.	6438.	6438.
$\Delta a = -\frac{f(a)}{f'(a)}$.008315	-0.0412	-0.063
Solution			0.578303

Similarly, - 26.8019 is found to be a solution. A method of finding the two

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VIII- [REDACTED]

other solutions was shown in Section 8.1-2. It is to be observed that there will necessarily be much cancellation in the computation of $f(a)$ since we wish it to be zero. Hence it may be necessary to carry this computation to many figures, taking a as exact (i.e., an exact number used as a trial value; of course it is not the exact solution).

On the other hand, $f'(a)$ will generally not involve much cancellation and only a few figures of it are needed for Δa ; indeed, once a has been found to a few figures, $f'(a)$ will be known closely enough and need not be recomputed. It may be remarked here that any fairly close approximation to $f'(a)$ may be used. This will not affect the fact that successive approximations converge to the answer, provided $f'(a)$ is not near zero, though it may make the convergence slower.

8.1-6 Checking Solutions

The test of the correctness of the solutions found is whether they satisfy the given equation.

An error in one step of either Newton's method or the method of successive interpolations, unless it is the last trial (which should essentially agree with the previous trial), will not vitiate the final answer but only result in slower convergence to that answer. A systematic error (the same mistake in each trial) may, on the other hand, lead to an incorrect result.

8.1-7 Choice of Method

While there are still other methods⁽⁹⁾, those outlined above are generally

(9)

Scarborough, loc. cit., Chapter X.

Whittaker and Robinson, loc. cit., Chapter VI.

adequate and satisfactory.

If $f'(x)$ can readily be found, and $f(x)$ and $f'(x)$ are not difficult to calculate numerically, Newton's Method (Section 8.1-5) is generally preferable.

[REDACTED]

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If $f'(x)$ is hard to find or much more difficult to compute numerically than $f(x)$, then the method of successive interpolation (Section 8.1-3) is preferable. The method of iteration has the advantage of involving a little less calculation at each step than the other methods, which is worthwhile if there is reason to suppose that one will not lose much in rapidity of convergence.

8.2 CURVE FITTING (BY LEAST SQUARES) (Whitman)

In fitting a curve to a set of values obtained by experimental methods, the theory of least squares is sometimes found useful. The general form of the problem of curve fitting is that several corresponding values of two variables are measured experimentally, an appropriate equation is assumed to give the relationship between the two variables, and then the parameters of the equation are determined.

The simplest type of equation to use is a polynomial. The degree of the polynomial can be determined by differencing the values of the dependent variable. If the second differences are fairly constant a parabola may be used for the approximating curve, if the third differences - a cubic, etc. Since some experimental error appears in each pair of measured values, one equation cannot fit all points exactly, but the method of least squares gives the optimum approximating curve⁽¹⁰⁾.

(10)

J. B. Scarborough, The Johns Hopkins Press, Numerical Math. Analysis (1930), p. 304 ff.

The theory consists of minimizing the error between the fitted polynomial and the points given by the experimental data by minimizing the sum of the squares of the errors at those points. Since both positive and negative errors are assumed to occur in such a way as to average out to zero, the squares of the errors must be used to insure an absolute numerical minimum.

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The theory is intended to minimize the actual error that occurs between the supposed or measured value and the true value; but since this error can never be determined in practice, the "residual" is found, i.e., the difference between the measured value of the dependent variable and the value of the function found from the computed parameters and the independent variable. It can be shown that minimizing the residuals is equivalent to minimizing the true errors.

To take a general example, suppose we have n pairs of values, (x_i, y_i) measured experimentally and we wish to fit a parabola to these points. We write

$$y_i^1 = A_1 + A_2 x_i + A_3 x_i^2 \quad (18)$$

using the notation y_i^1 to distinguish the computed values from the experimental values of y . The problem now is to solve for the A 's.

Writing y_i for y_i^1 in (18) and dividing the equation by y_i , we obtain

$$1 = A_1 \frac{1}{y_i} + A_2 \frac{x_i}{y_i} + A_3 \frac{x_i^2}{y_i} \quad (19)$$

We then multiply Equation (19) by the coefficient of each of the A 's, in turn, and sum the resulting equations, obtaining the set

$$\left\{ \begin{array}{l} \sum \frac{1}{y_i} = A_1 \sum \frac{1}{y_i^2} + A_2 \sum \frac{x_i}{y_i^2} + A_3 \sum \frac{x_i^2}{y_i^2} \\ \sum \frac{x_i}{y_i} = A_1 \sum \frac{x_i}{y_i^2} + A_2 \sum \frac{x_i^2}{y_i^2} + A_3 \sum \frac{x_i^3}{y_i^2} \\ \sum \frac{x_i^2}{y_i} = A_1 \sum \frac{x_i^2}{y_i^2} + A_2 \sum \frac{x_i^3}{y_i^2} + A_3 \sum \frac{x_i^4}{y_i^2} \end{array} \right. \quad (20)$$

These equations allow us to solve for the desired parameters (usually by rule of determinants), and we have the solution of our problem.

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That the Equations (20) give the required result can be shown theoretically,⁽¹¹⁾

(11) Whittaker and Robinson, Blackie and Son, Ltd. (1940) - The Calculus of Observations, p. 210-211.

and so this process does not appear in the numerical work. The theory, however, should be utilized whenever possible as a check on the numerical work. For instance, the residuals are easily computed by taking $r_i = y_i^1 - y_i$.

Hence, $\sum r_i$ can be computed directly. Also

$$\sum r_i \approx A_1 \sum \frac{1}{y_i} + A_2 \sum \frac{x_i}{y_i} + A_3 \sum \frac{x_i^2}{y_i} - \sum 1$$

The separate sums on the right appear in the existing computation, and so we have a simple check on the correctness of the calculations. One should expect to find that $\sum r_i = 0$, within the desired accuracy. The A's of course, may be checked by substitution in (20).

Another, more exacting check, is performed by taking the sums

$$\sigma_i = \frac{1}{y_i} + \frac{x_i}{y_i} + \frac{x_i^2}{y_i}$$

and also

$$\sum \frac{1}{y_i} \sigma_i, \sum \frac{x_i}{y_i} \sigma_i, \sum \frac{x_i^2}{y_i} \sigma_i$$

Then the following two equations form a check, since the left hand sums appear in the previous computation⁽¹²⁾.

(12) Whittaker and Robinson, Blackie and Son, Ltd. (1940) - The Calculus of Observations, p. 211.

$$\left\{ \begin{aligned} \sum \frac{x_i}{y_i} \cdot \frac{1}{y_i} + \sum \frac{x_i}{y_i} \cdot \frac{x_i}{y_i} + \sum \frac{x_i}{y_i} \cdot \frac{x_i^2}{y_i} &= \sum \frac{x_i}{y_i} \sigma_i \\ \sum \frac{x_i^2}{y_i} \cdot \frac{1}{y_i} + \sum \frac{x_i^2}{y_i} \cdot \frac{x_i}{y_i} + \sum \frac{x_i^2}{y_i} \cdot \frac{x_i^2}{y_i} &= \sum \frac{x_i^2}{y_i} \sigma_i \end{aligned} \right.$$

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If the residuals, r_i , are squared and summed, the sum should be near zero for a check on gross errors. It can also be shown⁽¹³⁾ that

(13)

Whittaker and Robinson, Blackie and Son, Ltd. (1940) - The Calculus of Observations, p. 234.

$$\sum r_i^2 = \sum y_i^2 - A_1 \sum y_i \cdot \frac{1}{y_i} - A_2 \sum y_i \cdot \frac{x_i}{y_i} - A_3 \sum y_i \cdot \frac{x_i^2}{y_i}$$

It may be that a certain "weight" should be attached to each observation so that instead of the points (x_i, y_i) we have $(w_i x_i, y_i)$. The points might simply be weighted according to position ($w_i = \frac{1}{y_i}$ or $w_i = \frac{1}{x_i}$). The residuals are affected linearly according to weight. The checks should be formed using the weighted residuals, for instance, the last formula would read

$$\begin{aligned} \sum w_i r_i^2 = & \sum w_i y_i^2 - A_1 \sum y_i \cdot \frac{w_i}{y_i} - A_2 \sum y_i \cdot \frac{w_i x_i}{y_i} \\ & - A_3 \sum y_i \cdot \frac{w_i x_i^2}{y_i} \end{aligned}$$

8.3 HARMONIC ANALYSIS (Flanders)

It is sometimes desirable to represent a periodic function $f(x)$ in the form

$$\begin{aligned} f(x) = & a_0 + a_1 \cos x + a_2 \cos 2x + a_3 \cos 3x + \dots + b_1 \sin x + b_2 \\ & \sin 2x + b_3 \sin 3x + \dots \end{aligned}$$

This subject has been exhaustively treated in studies of Fourier series; a good description of a practical method for finding the first few coefficients is given by Scarborough and Whittaker and Robinson⁽¹⁴⁾.

(14)

Scarborough, loc. cit., pp. 388-405.

Whittaker and Robinson, loc. cit., Chapter X, especially the insert facing p. 270.


8.4 GENERAL PROCEDURES IN "HAND" COMPUTATIONS

8.4-1 Setting Up Numerical Computations

When a mathematical problem is to be solved numerically, there are three principal parts to the job: "setting up" the problem, performing the calculations, and checking the results.

The setting up may be simply a matter of specifying the numerical operations to be performed, or it may require manipulation of the given formulas or equations to obtain a more convenient form. How detailed the specification of the operations must be depends upon the qualifications of the computer; a style suitable for computers with limited knowledge of mathematics is shown in Section 5.1-9, Chapter 5. For the sake of flexibility it is usually advisable to make the directions detailed enough to be readily intelligible to the least well-trained computer in a group. However, for some problems this is impracticable and they must be given to computers who can do the work without detailed instructions. In the process of setting up a problem, it is well to watch for things which look inconsistent (for instance, a regular procession of powers with one exception, or a certain combination of expressions repeated several times but once slightly different) and check their correctness with the person providing the problem.

In many cases, especially in numerical integration (Section 3.1, Chapter 3) the person who sets up a problem must also determine what values of the argument are to be substituted in formulas in order to achieve a specified accuracy in the answer or a suitable distribution of answers. In some cases an inspection of the formula will indicate the proper choice; in other cases, it is necessary to substitute a number of values of the argument and inspect the results to see whether more are needed. Similar remarks apply to the determination of the number of significant figures to be carried if the constants in the formulas

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are exact. It may be pointed out that it is usually advisable to carry an extra figure or two so as not to have to worry about rounding-off errors.

8.4-2 Carrying Out the Calculations

If the set up is adequate, the computation itself should be simple though perhaps tedious.

8.4-3 Checking the Calculations

Checking the work is the last item but by no means the least. The set up should be checked before starting computation; presumably this will be done by a person competent to judge the necessary technique so our remarks will be confined to the checking of the numerical work.

Basically there are two types of check: self-consistency of results, and comparison of two independent calculations.

Whether results are self-consistent may be determined by seeing whether the answers (for various values of the argument) run in smooth succession. Gross individual errors (but not systematic errors) may thus be detected at a glance; to detect smaller errors one may take the first, second or higher differences (Section 2.1-1) of the answers and inspect their regularity. The effect on the differences of an error in one value of the function may be seen from the following table. Thus, the first variation in the differences appears on the line where the error occurred, but the greatest variation is opposite a Z with greater subscript.

If it is observed that there is an error, but it is not apparent where this error lies, one may take differences of the terms or factors which enter directly into the computation of Z , and of the items which enter into these terms or factors, and so on. If the differences oscillate in one step A and not in the items which enter into A , then presumably the error lies in the computation of A .

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Z	$\Delta_1 Z$	$\Delta_2 Z$	$\Delta_3 Z$	$\Delta_4 Z$
Z_1				
Z_2	$\Delta_1 Z_2$			
Z_3	$\Delta_1 Z_3$	$\Delta_2 Z_3$		
Z_4	$\Delta_1 Z_4$	$\Delta_2 Z_4$	$\Delta_3 Z_4$	
Z_5	$\Delta_1 Z_5$	$\Delta_2 Z_5$	$\Delta_3 Z_5$	$\Delta_4 Z_5$
Z_{6+}	$\Delta_1 Z_{6+\epsilon}$	$\Delta_2 Z_{6+\epsilon}$	$\Delta_3 Z_{6+\epsilon}$	$\Delta_4 Z_{6+\epsilon}$
Z_7	$\Delta_1 Z_{7-\epsilon}$	$\Delta_2 Z_{7-2\epsilon}$	$\Delta_3 Z_{7-3\epsilon}$	$\Delta_4 Z_{7-4\epsilon}$
Z_8	$\Delta_1 Z_8$	$\Delta_2 Z_{8+\epsilon}$	$\Delta_3 Z_{8+3\epsilon}$	$\Delta_4 Z_{8+0\epsilon}$
Z_9	$\Delta_1 Z_9$	$\Delta_2 Z_9$	$\Delta_3 Z_{9-\epsilon}$	$\Delta_4 Z_{9-4\epsilon}$
Z_{10}	$\Delta_1 Z_{10}$	$\Delta_2 Z_{10}$	$\Delta_3 Z_{10}$	$\Delta_4 Z_{10+\epsilon}$
Z_{11}	$\Delta_1 Z_{11}$	$\Delta_2 Z_{11}$	$\Delta_3 Z_{11}$	$\Delta_4 Z_{11}$

It will be observed, for instance, from the above table that an error of one in the last digit in Z_6 (which might easily arise from rounding off) will cause an error of 6 in the last figure of $\Delta_4 Z_8$, as well as errors of opposite sign in adjacent values of $\Delta_4 Z$, so this much variation in $\Delta_4 Z$ is not significant.

Even though the differences indicate no error, the computation should be done independently for at least one value of the argument, to guard against systematic errors.

In some cases the check of self-consistency is not applicable; for instance, if there are too few values of the argument the differences of the answers will not afford a sufficient test; if the values of the argument are not equally spaced, it is difficult to get adequately comparable differences (15).

(15)

However, something along this line can be done by the use of "divided differences"; cf. E. T. Whittaker and G. Robinson, The Calculus of Observations, p. 20.

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The other method of checking is to make two independent computations, using either two different computers or two different methods; the latter alternative is in some respects theoretically more attractive, but the former is usually more practical.

In order to obtain really "independent" computations by two computers, it is best to have them work without communicating with each other with a third person comparing the results, finding the source of any discrepancies, and returning incorrect work to the computer for correction. However, this procedure may not always be practical and it may be necessary to allow the computers to compare figures now and then to avoid further computation with incorrect values. This involves some danger that one will convince the other of the correctness of an incorrect value or operation; the extent of the danger depends on the character of the computers.

To minimize time spent in checking one may, in setting up a problem, specify the recording of values at intermediate steps rather than only the recording of the final answer to a complicated computation; also, one may indicate points at which a check should be made before continuing.

A method intermediate between self-consistency and computation by two independent methods is that used in checking step-by-step integration of differential equations (Section 5.1-3, Chapter 5). Here one computes a new value on the basis of the old ones, then substitutes the "new value" into a formula which should yield the same "new value" over again; failure to do so indicates a mistake.

8.4-4 Other Items

A few odds and ends in the way of practical considerations may be mentioned.

All work sheets should be labelled so that they can be identified months later when memory is dulled.

A person who gives the computing group a job may not have much idea what

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he wants in the way of accuracy; if so, it is better to do a fairly accurate job the first time instead of having to do it over again.

When a great many values of a very complicated function must be used in computations, it is convenient to calculate chosen values of the function and to draw a graph. The values are chosen so that they are simple to compute with and also so that the curve is sufficiently well defined, e.g., a hump in the curve requires more points than would a fairly linear segment. The computed points are then plotted and the scale chosen large enough to allow the desired number of significant figures to be read from the graph. A small amount of accuracy may be sacrificed in this method, but a great mass of detailed computing is obviated.

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