



A HEAT FLOW PROBLEM IN ELECTRON BEAM ETCHING
OF THIN FILMS

by

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ABSTRACT

As the problems of modern science and technology become more complex, the need arises for digital computers of greatly increased speed and storage capacity. Previous work has indicated that computer components may be made from thin metallic films, and that the possible switching times of such components may be such that the overall speed of the computer will be limited by the transit time of a signal from one part of the computer to another, rather than by the speed of the components themselves. In order to fully exploit the speed of such components, while maintaining large computer storage capacity, it becomes necessary to pack a very large number of components into a small volume.

One approach to miniaturization is to etch components and circuits in a thin film by heating microscopic regions of the film to evaporation temperatures with an electron beam. This thesis presents a study of the heat flow problem, which is simplified to the problem of finding the temperature rise on a thin plate, with a uniform circular source of heat in uniform rectilinear motion on the plate. The temperature was found as a function of position and velocity in terms of a double integral. An IBM 704 computer program was written to perform the numerical evaluation of the integral.

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I. Introduction

The modern high-speed digital computer has been invaluable in dealing with the complex problems of modern science and technology. Not only have computers immensely shortened the time required to perform laborious and tedious mathematical and logical operations, they have also made possible the solution of problems which were heretofore insoluble in practice because of the great amount of time required to perform calculations. As problems of increasing complexity arise, however, it is found that computers of greater speed and storage capacity are needed.

Considerable research is being done at present toward the development of ultra high-speed computer components. Efforts to find ways of making such components from thin metallic films have shown considerable promise of success. Memory planes composed of thin films of ferromagnetic materials, and thin film versions of the cryotron, a superconducting switching device, are examples of components that seem feasible.

Work at M. I. T., and elsewhere, has indicated that switching times approaching 10^{-9} seconds may be possible in some of these devices. When switching speeds of this order of magnitude are attained, the speed of a computer becomes limited by time required for a signal to propagate from one part of the computer to another. If the computer is to have both high speed and large storage capacity, it then becomes necessary not only to increase the switching speed of the individual components, but also to miniaturize the components and circuits so that the distance through which a signal must travel between cycles is short.

One approach to miniaturization is to make components and circuits by etching a uniform thin film in such a way the desired geometry results — a sort of "printed circuit" technique in miniature. Such a procedure is under investigation at the M. I. T. Digital Computer Components and Systems Group (DCCSG). It involves the projection of an electron beam image of the desired

configuration on the film. The electron optics are such that the image is greatly reduced in size, so that complex configurations may be projected on a very small area. The electron beam seems to catalyze a reaction in the residual gasses in the vacuum system, causing a carbonaceous deposit to appear on the film in regions of high beam intensity. After a deposit of suitable thickness has been formed, the electron beam is turned off, and a corrosive gas, such as chlorine, is admitted to the system. The gas reacts with the portions of the metallic film which are not protected by the carbonaceous deposit causing them to be etched away. The deposit and the products of the etching reaction may then be removed, leaving the desired configuration in the film.

The above process, however, has the disadvantage that foreign gasses must be admitted to the vacuum system. This could be very troublesome in many instances, especially if the same system is used for the formation of the film by evaporation. If films of high purity are to be made, the requirements for good vacuum are quite stringent, so that any contamination of the vacuum system is to be avoided if possible.

An alternative method is suggested of etching the film without having to contaminate the vacuum system. If an electron beam of sufficient intensity could be focussed upon the film, it is expected that enough heat would be produced in the film to cause sublimation or vaporization to take place in the locality of the beam. The beam could be deflected to scan repeatedly over the regions of the film to be removed, until evaporation had removed all of the undesired material. Such a system could be a powerful tool in the construction of computer circuits, for the configuration of the circuitry would be under electronic control, hence adaptable to methods of automation. The further possibility suggests itself of placing the entire system under the control of a computer, so that the computer would both design and build the circuit, thereby producing highly complex logical circuits with a minimum of human effort.

The topic of this thesis is the study of the heat flow problem in the film as it is bombarded by the scanning electron beam, to determine the feasibility of using such a method to evaporate parts of the film. Some simplifications are made, as explained in the next chapter, to obtain at least a first approximation of the conditions to be expected. The heat flow problem is reduced to the problem of finding the temperature distribution over a conducting plane which contains a circular heat source in uniform rectilinear motion, emitting heat at a constant rate, uniformly over its area. Although the immediate application of this study is directed toward the electron beam scanning problem, it is possible that practical applications may exist elsewhere, such as the arc welding of flat plates, machining or buffing of plates, etc.

CHAPTER II

II. Nature of the Problem

It would be desirable to develop a system which can etch configurations on films to a tolerance approximately equal to the film thickness, which is of the order of a few hundred to a few thousand Angstroms. This places rather stringent requirements on the electron focussing system, for the beam must be focused down to a diameter of the order of 1000 Angstroms, and yet have sufficient intensity to heat the film to a temperature of vaporization or sublimation. Moreover, the energy of the electrons in the beam is limited to a point where most of the electrons penetrate completely through the film. According to Whiddington's law, if the energy of the electrons is further increased, the energy which they lose to the film, when passing through it, will decrease. It is expected that the optimum energy will be of the order of a few thousand electron volts. It therefore becomes necessary to increase the current of the beam in order to increase its heating effect upon the film. It is, however, quite difficult to produce an electron gun which will focus a high current electron beam to a diameter of 1000 Angstroms. The objective of this thesis is the determination of the scanning velocity and quantity of heat required to produce a suitable temperature distribution on the film, so that the feasibility of using an electron beam to heat the film to sublimation or vaporization temperatures may be accurately evaluated. It is expected that a compromise will have to be found between a high scanning velocity, which would give a temperature distribution such that the film temperature in the path of the beam is relatively high but falls off rapidly at positions away from beam's path, and a low scanning velocity, which would give a more uniform temperature, but would give a higher maximum temperature for the same beam current, due to the fact that the beam remains in a given region for a longer period of time. The temperature difference between a point in the path of the beam and a nearby point outside the path of the beam should be as great as is practical, so that the sublimation or vaporization of the film will occur only in the desired locations.

In order to find an approximate solution of the heat flow problem, certain simplifying assumptions will be made. It is assumed that a metallic film is deposited upon a substrate of much lower thermal conductivity, such as glass. The scanning electron beam moves in a straight line at constant velocity. As the beam repeatedly scans a line in the film it is assumed that the time between scans is sufficient for the region under consideration to reach a uniform temperature. The current density of the focused beam—the number of electrons crossing a unit cross-section area per unit time—is assumed to be constant within the beam diameter, and zero outside. This will not be the case in practice, but the results from this assumption are expected to provide a first approximation. Moreover, results of better accuracy may be found by superimposing uniform beams of differing diameters to attain an approximation of the true current density distribution. The temperature distribution on the film may then be approximated by superimposing the temperature distributions for the uniform beams.

It is also assumed that the density, thermal conductivity, and thermal capacity of the film remain constant as temperature varies. This is not strictly true in practice, for these "constants" may vary by as much as twenty or thirty percent for temperature changes of 100°C . Even larger variations are to be expected as the melting point of the film is approached. Moreover, film constants, such as these, are very difficult to measure accurately, for they differ in general from the constants of the material in bulk form. It is again expected, however, that a reasonably good first approximation may be found by assuming bulk characteristics, and by assuming that they do not vary with temperature.

Finally, it will be assumed that the temperature is uniform through the thickness of the film, so that two dimensional geometry may be used, and that no heat is lost from the surfaces of the film. Heat will be conducted away from the film by the substrate, in practice, but the thermal conductivity of the film will probably be of the order of 100 to 1000 times greater than that of the substrate, so that the heat lost to the substrate in the immediate region of the source is expected to be negligible, to a first approximation. It is important to note, however, that if the focused diameter of the electron beam

is large in comparison to the film thickness, this assumption becomes invalid.

The problem, then, is reduced to finding the temperature distribution on a conducting plane that contains a uniform circular heat source moving in a straight line at constant velocity. This problem will be solved explicitly in terms of a double integral in the next chapter. A program for an IBM 704 computer has been written to perform numerical evaluations of this solution.

III. Derivation of the Equations

The Heat Flow Equation

The temperature at any point in an isotropic homogenous medium is governed by the well-known heat flow equation:

$$\frac{\partial U}{\partial t} = a^2 \nabla^2 U + \frac{1}{\rho C} F(x, y, t) \quad (3-1)$$

where

U = temperature

t = time

a^2 = thermal diffusivity

$$= \frac{k}{\rho C}$$

k = heat conductivity of the medium

ρ = density of the medium

C = thermal capacity of the medium

∇^2 = the Laplacian operator

F(x, y, t) = heat supplied to the medium from a source

It will be convenient here to consider the case where F(x, y, t) is identically zero.

$$\frac{\partial U}{\partial t} = a^2 \nabla^2 U \quad (3-2)$$

Since equation (3-2) is linear, it follows that a linear combination of solutions is also a solution; the principle of superposition holds.

In this thesis, attention will be restricted to solutions of this equation in two dimensions. Equation (3-2) when written in terms of cartesian coordinates becomes

$$\frac{\partial U}{\partial t} = a^2 \left(\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} \right) \quad (3-3)$$

and, in polar coordinates:

$$\frac{\partial U}{\partial t} = a^2 \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial U}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 U}{\partial \theta^2} \right] \quad (3-4)$$

Equation (3-4) applies, in particular, to a flat plate parallel to the x-y plane, provided there is no variation in temperature in the plate along any line perpendicular to the x-y plane, and provided no heat is lost from the surfaces of the plate. If the plate is of thickness d , and is composed of material whose bulk heat conductivity is k' , whose bulk density is ρ' , and whose bulk thermal capacity is C' , the constants in equation (4) are given as follows:

$$\begin{aligned} k &= d k' \\ \rho &= d \rho' \\ C &= d C' \\ a^2 &= \frac{k}{\rho C} = \frac{1}{d} \frac{k'}{\rho' C'} = \frac{1}{d} (a')^2 \end{aligned}$$

where $(a')^2$ is the thermal diffusivity in the three dimensional problem.

The Source Functions of Heat Flow

If a^2 is constant, as will be assumed throughout this thesis, a solution of equation (3-4) which has some useful properties is the heat source function:

$$U = \frac{q}{4\pi\rho Ca^2 t} e^{-\left(\frac{s^2}{4a^2 t}\right)} \quad (3-5)$$

This function (3-5) may be interpreted, for positive t , as the temperature on a plane at distance s from the origin due to a quantity of heat, q , suddenly released at the origin at time $t = 0$.

The surface integral of the source function over the entire plane is equal to q/C , independent of t , satisfying the requirement that heat be conserved. The function is finite and positive everywhere when t is greater than zero, it is zero everywhere when $t = 0$, except at the origin, where it goes to infinity, if we take the limit in such a way that the surface integral over the plane remains continuous.

The source functions for one- and three-dimensional geometries are listed here for reference:

one dimension (point source on a line)

$$U = \frac{q}{\rho C} \frac{1}{(4\pi a^2 t)^{1/2}} e^{-\left(\frac{s^2}{4a^2 t}\right)} \quad (3-6)$$

satisfies: $\frac{\partial U}{\partial t} = a^2 \frac{\partial^2 U}{\partial x^2}$ $s^2 = x^2$

three dimensions (point source in a solid)

$$U = \frac{q}{\rho C} \frac{1}{(4\pi a^2 t)^{3/2}} e^{-\left(\frac{s^2}{4a^2 t}\right)} \quad (3-7)$$

satisfies: $\frac{\partial U}{\partial t} = a^2 \left(\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2} \right)$

where $s^2 = x^2 + y^2 + z^2$

s = the distance between the source and the point of observation

It will be convenient to normalize time and quantity of heat as follows:

$$T = 4 a^2 t \quad (3-8)$$

$$Q = \frac{q}{\rho C} \quad (3-9)$$

where

t = real time

T = normalized time

q = real quantity of heat

Q = normalized quantity of heat.

The use of normalized quantities in the following equations removes the dependence upon the properties of the material, thereby simplifying the equations considerably. Hereafter, unless real quantities are specified, any mention of heat and time will be assumed to refer to the normalized quantities. This convention will also apply to quantities which are defined in terms of heat or time. A normalized velocity V , for example, will be related to the real velocity v as follows:

$$V = \frac{dx}{dT} = \frac{1}{4a^2} \frac{dx}{dt} = \frac{1}{4a^2} v \quad (3-10)$$

A normalized time rate of heat flow P will be related to the real rate of heat flow p as:

$$P = \frac{dQ}{dT} = \frac{1}{4a^2 \rho C} \frac{dq}{dt} = \frac{1}{4a^2 \rho C} p = \frac{1}{4k} p \quad (3-11)$$

The source functions in one, two, and three dimensions (equations 3-6, 3-5, and 3-7, respectively), when written in terms of normalized quantities become;

$$\text{one dimension:} \quad U = \frac{Q}{(\pi T)^{1/2}} e^{-\frac{s^2}{T}} \quad (3-12)$$

two dimensions:

$$U = \frac{Q}{\pi T} e^{-\frac{s^2}{T}} \quad (3-13)$$

three dimensions:

$$U = \frac{Q}{(\pi T)^{3/2}} e^{-\frac{s^2}{T}} \quad (3-14)$$

The source function (3-13) and the principle of superposition permit us to express in integral form the temperature at any location on the plane at any time, for a heat source which may be an arbitrary function of both position and time. Let $G(x, y, T)$ be such a function, defined as follows:

$$G(x, y, T) = \lim_{\substack{\Delta S \rightarrow 0 \\ \Delta T \rightarrow 0}} \frac{P_a(x, y, T)}{\Delta S \Delta T}$$

where P_a is the amount of normalized heat supplied to the incremental area ΔS at location (x, y) in the increment of normalized time from T to $T + \Delta T$. We may now rewrite equation (3-13), replacing Q by the heat contributed by the source to a differential area dS , in a differential time dT .

$$dU = \frac{G(x, y, T)}{\pi T} e^{-\frac{x^2 + y^2}{T}} dx dy dT$$

The differential temperature at the point (X, Y) at time W is then given by;

$$dU = \frac{G(x, y, T)}{\pi(W - T)} e^{-\frac{(X-x)^2 + (Y-y)^2}{W - T}} dx dy dT$$

remembering that T in equation (3-13) refers to the elapsed time between the emission of the heat and measurement of the temperature, and s refers to the distance from the source to the point of measurement.

We may now integrate over the entire plane, and over time, to obtain the temperature due to the entire source $G(x, y, T)$:

$$U = \frac{1}{\pi} \int_{-\infty}^W \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{G(x, y, T)}{W-T} e^{-\frac{(X-x)^2 + (Y-y)^2}{W-T}} dx dy dT \quad (3-15)$$

Equation (3-15) gives the temperature at any point (X, Y, Z) , at any time W , on a plane which contains an arbitrary heat source described by $G(x, y, T)$.

Consider now the case of a point source moving in a straight line at a constant velocity V (as defined in 3-10). Let the normalized rate of heat emission be P_p (see 3-11), and let the source move in a positive direction on the x axis from $x = -\infty$ so that it coincides with the origin at time $T = 0$.

If we introduce the variable:

$$z = x - VT \quad (3-16)$$

the function $G(x, y, T)$ will be given by:

$$G(x, y, T) = P_p \delta(y, z)$$

where $\delta(y, z)$ is an impulse function defined by:

$$\left. \begin{aligned} \delta(y, z) &= 0 \quad \text{when } y^2 + z^2 \neq 0 \\ \delta(y, z) &= \infty \quad \text{when } y^2 + z^2 = 0 \end{aligned} \right\} \quad (3-17)$$

$$\int_{-\epsilon}^{\epsilon} \int_{-\epsilon}^{\epsilon} \delta(y, z) dy dz = 1$$

Substituting into equation (3-15) for x and $G(x, y, T)$, it is found that:

$$U = \frac{P_p}{\pi} \int_{-\infty}^W \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\delta(y, z)}{W-T} e^{-\frac{(X-z-VT)^2 + (Y-y)^2}{W-T}} dz dy dT \quad (3-18)$$

Reference to (3-17) shows that:

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \delta(y, z) F(y, z) dy dz = F(0, 0)$$

provided $F(y, z)$ is continuous at $y = z = 0$. Therefore:

$$U = \frac{P}{\pi} \int_{-\infty}^W \frac{1}{W-T} e^{-\frac{(X-VT)^2 + Y^2}{W-T}} dT \quad (3-19)$$

Substitution of the variables:

$$Z = X - VW \quad (3-20)$$

$$a = W - T$$

yields:

$$U = \frac{P}{\pi} e^{-2VZ} \int_0^{\infty} \frac{1}{a} e^{-\left(\frac{Z^2 + Y^2}{a} + V^2 a\right)} da \quad (3-21)$$

Now let:

$$Y^2 + Z^2 = R^2 \quad (3-22)$$

$$\beta = 2V^2 a$$

and equation (3-21) becomes:

$$U = \frac{P}{\pi} e^{-2VZ} \int_0^{\infty} \frac{1}{\beta} e^{-1/2\left(\beta + \frac{4V^2 R^2}{\beta}\right)} d\beta \quad (3-23)$$

It can be shown that:*

$$K_n(Z) = \frac{Z^n}{2} \int_0^{\infty} \beta^{-n-1} e^{-1/2\left(\beta + \frac{Z^2}{\beta}\right)} d\beta \quad (3-24)$$

* See, for example, Reference 20, Chapter 5.

where $K_n(z)$ is the modified Hankel function (also known in the literature as the modified Bessel function of the second kind, modified Bessel function of the third kind, and Basset's function).

In particular:

$$K_0(z) = \frac{1}{2} \int_0^{\infty} \frac{1}{\beta} e^{-\frac{1}{2}\left(\beta + \frac{z^2}{\beta}\right)} d\beta \quad (3-25)$$

Substituting (3-25) into (3-23):

$$U_p = \frac{2P}{\pi} e^{-2VZ} K_0(2VR) \quad (3-26)$$

which gives the temperature at any point in the plane containing a moving point source of heat.

From (3-20) and (3-22):

$$Z = X - VW \quad (3-27)$$

$$R = (Y^2 + Z^2)^{1/2} \quad (3-28)$$

Reference to the normalizing equations (3-10) and (3-11) shows that the parameters of equation (3-26) may be expressed in terms of real physical quantities as follows:

$$V = \frac{1}{4a^2} v \quad (3-29)$$

$$P_p = \frac{1}{4a^2 \rho C} P_p = \frac{1}{4k} P_p \quad (3-30)$$

$$Z = X - VW = X - vt \quad (3-31)$$

Examination of equation (3-26) shows the following properties. If a surface is plotted of the temperature U as a function of the coordinates X and Y (Figure 1), and its behavior observed as time is varied, it will be seen that the shape of the surface remains unchanged, but that the entire surface moves in the positive X direction at the same velocity as the source (this is true whether the velocities and times considered are normalized or real physical quantities). The geometrical relationship between the temperature surface and the source remains unchanged in time. This property is quite helpful in the physical interpretation of equation (3-26), for it permits the elimination of any explicit dependence of the temperature on time. The variables Z and Y correspond to the coordinates in a cartesian plane moving at the same velocity as the source. The source is at the origin of the Z - Y plane, and moves, with the X - Y plane, in the direction of the positive Z axis. The variable R , then, becomes the distance from the origin to the point of observation.

A rather interesting property of equation (3-26) is its dependence only upon the variables (VZ) and (VR) , so that only two independent variables are required to describe the behavior of the function. If the temperature surface is plotted for a particular value of V , the surface for smaller or larger V will be obtained if this surface is expanded or contracted, respectively, uniformly in the Z - Y plane, in inverse proportion to the change in V .

The temperature (equation 3-26) is given by the product of a function of R and a function of Z . Hence, it can be visualized as the "product" of a surface of revolution whose axis goes through the origin perpendicular to the Z - Y plane, and an exponential cylinder parallel to the Y axis. The surface of revolution is described by the function $K_0(2VR)$, the modified Hankel function. For a real positive argument, this function has a logarithmic singularity at the point zero, and decreases monotonically to zero as the argument goes positive to infinity.

As $(2VR)$ becomes small, the function can be represented asymptotically by:

$$K_0(2VR) \sim -\ln(VR) \xrightarrow{VR \rightarrow 0} + \infty \quad (3-32)$$

For large $(2VR)$, the asymptotic representation is as follows:

$$K_0(2VR) \sim \sqrt{\frac{\pi}{4VR}} e^{-2VR} \xrightarrow{VR \rightarrow \infty} 0 \quad (3-33)$$

It will be noted from equation (3-26) that for constant V and R , the maximum temperature will be found on the negative Z axis. If the temperature is observed on the Z axis as Z goes toward $-\infty$, (constant V), it is found by substitution of (3-33) into (3-26) that the exponentials cancel, and the temperature approaches the following asymptotic representation:

$$U \sim P_p \sqrt{\frac{1}{\pi VR}} \xrightarrow{VR \rightarrow \infty} 0 \quad (3-34)$$

The temperature therefore approaches zero as R becomes very large in any direction.

Uniform Circular Source

Consider now the case of a circular source of unit radius, centered at the origin of the Z - Y plane, whose rate of heat emission per unit area is P_c inside the unit circle, and zero outside. The temperature observed at the point $(Z = A, Y = B)$ due to the heat emitted from a differential area dS at the point (Z_1, Y_1) is, from equation (3-26):

$$dU_c = \frac{2}{\pi} P_c e^{-2V(A-Z_1)} K_0 \left[2V \sqrt{(A-Z_1)^2 + (B-Y_1)^2} \right] dS$$

The temperature from the circular source is found by integrating over the area covered by the source:

$$U_c(A, B) = \frac{2}{\pi} P_c e^{-2VA} \int_S e^{2VZ_1} K_0 [2V\sqrt{(A-Z_1)^2 + (B-Y_1)^2}] dS \quad (3-35)$$

where the integration is carried out over the interior of the circle:

$$Z_1^2 + Y_1^2 = 1$$

For purposes of machine computation, it is convenient to express the above integral as follows:

$$U_c = \frac{2}{\pi} P_c e^{-2VA} \int_{-1}^1 \sqrt{1-Y_1^2} \int_{-1}^1 e^{2V\sqrt{1-Y_1^2}\omega} K_0 [2V\sqrt{(A^2 + B^2 + Y_1^2 - 2BY_1) - 2A\sqrt{1-Y_1^2}\omega + (1-Y_1^2)\omega}] d\omega dY_1$$

where the substitution

$$\omega = \frac{Z_1}{\sqrt{1-Y_1^2}} \quad (3-37)$$

has been made.

It is helpful to note that (3-35), consequently (3-36) are equivalent to the surface integral of (3-26) over a circular region of unit radius whose center is at the point (A, B). The temperature due to a moving uniform circular source may therefore be visualized as being proportional to the volume enclosed by the following three surfaces: 1) the surface described by (3-26), which depicts the temperature from a moving point source located at the origin of the Z-Y plane, 2) a right circular cylinder of unit radius whose axis is perpendicular to the Z-Y plane and passes through the point of observation (A, B), and 3) the Z-Y plane itself (See Figure 12).

A Special Case

The temperature due to a uniform circular source may be found in terms of known functions in the special case:

$$A = B = 0 \quad (3-38)$$

In this case, the point of observation is at the center of the source in the Z-Y plane. The cartesian coordinates (Z_1, Y_1) in the integral of equation (3-25) may be replaced by polar coordinates (r, θ) by the usual transformations:

$$Z_1 = r \cos \theta, \quad Y_1 = r \sin \theta \quad (3-39)$$

from which:

$$r^2 = Y_1^2 + Z_1^2 \quad (3-40)$$

The differential area becomes:

$$dS = r \, d\theta \, dr \quad (3-41)$$

Substitution of (3-38), (3-40), and (3-41) into (3-35) yields:

$$U_c(0,0) = \frac{2}{\pi} P_c \int_0^1 r K_0(2Vr) \int_{-\pi}^{\pi} e^{2Vr \cos \theta} \, d\theta \, dr \quad (3-42)$$

The integral in θ can be shown to be expressible in terms of the modified Bessel function of the first kind, I_0 , as follows*:

$$I_0(2Vr) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{2Vr \cos \theta} \, d\theta \quad (3-43)$$

*See Reference 20, Chapter 5.

Equation (3-42) may therefore be written as follows:

$$U_c(0,0) = 4 P_c \int_0^1 r K_0(2Vr) I_0(2Vr) dr \quad (3-44)$$

(It may be noted that if the integration sign is removed from (3-34), the resulting equation gives the temperature at the center of a moving ring source of radius r :

$$U_r(0,0) = 4 P_r r K_0(2Vr) I_0(2Vr) \quad (3-45)$$

where P_r = rate of heat flow per unit length from the circumference or the ring source)

It is easily shown that the following equation holds:

$$\int x K_0(ax) I_0(ax) dx = \frac{x^2}{2} [I_0(ax) K_0(ax) + I_1(ax) K_1(ax)] \quad (3-46)$$

this may be verified by differentiation of the right hand side, using the formulas:

$$\frac{d}{dx} [x^\nu K_\nu(x)] = -x^\nu K_{\nu-1}(x) \quad (3-47)$$

$$\frac{d}{dx} [x^\nu I_\nu(x)] = x^\nu I_{\nu-1}(x) \quad (3-48)$$

and the properties:

$$I_{-n}(z) = I_n(z), \quad K_{-\nu}(z) = K_\nu(z) \quad (3-49)$$

(These, and other properties of modified Bessel functions are discussed more fully in Chapter 4.)

Equation (3-44) may be expressed, with the help of (3-46), as:

$$U_c = 2 P_c r^2 [I_0(2Vr) K_0(2Vr) + I_1(2Vr) K_1(2Vr)] \Big|_0^1 \quad (3-50)$$

Evaluation of this function at $r = 0$ produces an indeterminate result, for the functions K_0 and K_1 are infinite at this point, while the functions r^2 and I_1 are both zero. It is shown in chapter 4, however, that the limit of the function to be evaluated in (3-50) is zero, as r approaches zero.

Equation (3-50) then becomes:

$$U_c = 2 P_c [I_0(2V)K_0(2V) + I_1(2V)K_1(2V)] \quad (3-51)$$

(Source of unit radius)

This result may be generalized somewhat by noting that if the radius of the source is F_r , rather than unity, the integration in (3-44) will be carried out from zero to F_r . Hence, by (3-50):

$$U_c(F_r) = 2P_c F_r^2 [I_0(2VF_r) K_0(2VF_r) + I_1(2VF_r) K_1(2VF_r)] \quad (3-52)$$

Equation (3-52) will be found useful in evaluating the temperature at points inside the uniform circular source where A and B are not both zero. The numerical evaluation of equation (3-35) or (3-36) leads to difficulty in the region because of the singularity of the integrand at the point:

$$Z_1 = A, \quad Y_1 = B$$

Summary of the Equations

Recapitulating, the temperature at point (A, B) due to a point source moving at velocity V, with rate of heat emission P_p (normalized) is, from (3-26):

$$U_p(A, B, V, P_p) = P_p \frac{2}{\pi} e^{-2VZ} K_0(2VR) \quad (3-53)$$

where: $R = \sqrt{A^2 + B^2}$

The temperature at (A, B) due to a uniform circular source of unit radius centered at the origin, emitting heat at the rate P_c per unit area is, from (3-35):

$$U_c(A, B, V, P_c) = P_c \frac{2}{\pi} e^{-2VA} \int_S e^{2VZ_1} K_0[2V\sqrt{(A-Z_1)^2 + (B-Y_1)^2}] dS \quad (3-54)$$

where the integration is carried out over the Z_1 - Y_1 plane on the interior of the circle:

$$Z_1^2 + Y_1^2 = 1$$

If the total amount of heat emitted by the circular source per unit time (normalized) is P_t , equation (3-54) may be written:

$$U_t(A, B, V, P_t) = 2 P_t e^{-2VA} \int_S e^{2VZ_1} K_0[2V\sqrt{(A-Z_1)^2 + (B-Y_1)^2}] dS \quad (3-55)$$

for the total heat emission per unit time is:

$$P_t = S P_c = \pi r^2 P_c = \pi P_c$$

If $A = B = 0$, equation (3-54) reduces to (3-51):

$$U_c(0, 0, V, P_t) = 2 P_c [I_0(2V) K_0(2V) + I_1(2V) K_1(2V)] \quad (3-56)$$

and (3-55) becomes:

$$U_t(0, 0, V, P_t) = 2 \pi P_t [I_0(2V) K_0(2V) + I_1(2V) K_1(2V)] \quad (3-57)$$

The normalized parameters, P and V , are related to the real physical quantities p and v as follows:

$$\text{real rate of heat emission} = p_a = 4 k P_a$$

$$\text{real velocity} = v = \frac{4 k}{\rho C} V$$

The constants k, ρ , and C , are related to the bulk characteristics of the material, k', ρ' , and C' , by:

$$k = d k'$$

$$\rho = d \rho'$$

$$C = d C'$$

where d is the thickness of the material.

In the more general case where the radius of the source is F , rather than unity, a suitable change of variables in (3-35) leads to the following relations. Denoting by primes the temperatures due to the source of radius F :

$$U_c'(A, B, F, V, P_c) = U_c\left(\frac{A}{F}, \frac{B}{F}, VF, F^2 P_c\right) \quad (3-58)$$

c.f. (3-52)

$$U_t'(A, B, F, V, P_t) = U_t\left(\frac{A}{F}, \frac{B}{F}, VF, P_t\right) \quad (3-59)$$

IV. Modified Bessel Functions

A short discussion of modified Bessel functions is given here, and it is shown how the use of their properties leads to certain limiting expressions for the solutions of the moving source problem which were derived in the last chapter.

Bessel functions may be regarded as solutions of the differential equation:

$$z^2 \frac{d^2 w}{dz^2} + z \frac{dw}{dz} + (z^2 - p^2) w = 0 \quad (4-1)$$

This is a second order ordinary differential equation, hence it has two linearly independent solutions. One solution can be expressed as a power series, and is known as the bessel function of the first kind of order p :

$$J_p(z) = \sum_{m=0}^{\infty} (-1)^m \frac{(z/2)^{2m+p}}{m! \Gamma(m+p+1)} \quad (4-2)$$

where $\Gamma(x)$ is the generalized factorial function:

$$\Gamma(x) = \int_0^{\infty} t^{x-1} e^{-t} dt$$

$$\Gamma(x+1) = x\Gamma(x)$$

$$\Gamma(n+1) = n!$$

A second solution of (4-1) is found to be:

$$N_p(z) = \frac{1}{\sin(p\pi)} [J_p(z) \cos(p\pi) - J_{-p}(z)] \quad (4-3)$$

p not an integer

In the case where p is an integer n , (4-3) becomes indeterminate, and the function $N_n(z)$ is defined as the limit of (4-3) as p approaches n . The function $N_p(z)$ is known as the Bessel function of the second kind, or Neumann's function.

The Hankel functions, or Bessel functions of the third kind, are found useful in certain applications, and are given as follows:

$$H_p^{(1)}(z) = J_p(z) + i N_p(z)$$

$$H_p^{(2)}(z) = J_p(z) - i N_p(z) \quad (4-4)$$

$$i = \sqrt{-1}$$

If z is replaced by iz , Bessel's equation (4-1) becomes:

$$z^2 \frac{d^2 w}{dz^2} + \frac{dw}{dz} - (z^2 + p^2) w = 0 \quad (4-5)$$

Two linearly independent solutions of (4-5) are $I_p(z)$, and $K_p(z)$ -- the modified Bessel function of the first kind, and the modified Hankel function. $K_p(z)$ is also referred to in the literature as the modified Bessel function of the second kind, modified Bessel function of the third kind, and Basset's function.

The modified Bessel functions $I_p(z)$ and $K_p(z)$ are given as follows:

$$I_p(z) = \sum_{m=0}^{\infty} \frac{(z/2)^{2m+p}}{m! \Gamma(m+p+1)} \quad (4-6)$$

and:

$$K_p(z) = \frac{\pi}{2 \sin(p\pi)} [I_{-p}(z) - I_p(z)] \quad (4-7)$$

p not an integer

$I_p(x)$ and $K_p(x)$ are real when p is real and x is real and positive.

For the case $p = n$, an integer, $K_n(z)$ is defined as the limit of (4-7) as p approaches n , and becomes:*

$$K_n(z) = (-1)^{n+1} I_n(z) \ln(z/2) + 1/2 \sum_{m=0}^{n-1} (-1)^m (z/2)^{2m-n} \frac{(n-m-1)!}{m!} + \frac{1}{2} (-1)^n \sum_{m=0}^{\infty} (z/2)^{2m+n} \frac{\Psi(m+n+1) + \Psi(m+1)}{m! (m+n)!} \quad (4-8)$$

where $\Psi(x)$ is the logarithmic derivative of the gamma function:

$$\Psi(x) = \frac{d \ln \Gamma(x)}{dx}$$

In the case where x is a positive integer, $\Psi(x)$ can be expressed as follows:

$$\begin{aligned} \Psi(1) &= -\Upsilon \\ \Psi(n+1) &= 1 + 1/2 + 1/3 + \dots + 1/n - \Upsilon \end{aligned} \quad (4-9)$$

where Υ is Euler's or Mascheroni's constant:

$$\Upsilon = \lim_{m \rightarrow \infty} \left(\sum_{n=1}^m \left(1/n - \ln m \right) \right) = 0.577\ 215\ 664\ 9 \dots$$

From (4-6) and (4-7) it is seen that:

$$\begin{aligned} I_{-n}(z) &= I_n(z) \\ K_{-p}(z) &= K_p(z) \end{aligned} \quad (4-10)$$

* If $n=0$, the first summation in (4-8) becomes identically zero.

Term by term differentiation of (4-6) shows that:

$$\frac{d}{dz} [z^p I_p(z)] = z^p I_{p-1}(z) \quad (4-11)$$

$$\frac{d}{dz} [z^p K_p(z)] = -z^p K_{p-1}(z) \quad (4-12)$$

The modified Bessel functions of real argument x , $I_n(x)$ and $K_n(x)$, are related to ordinary Bessel functions as follows:

$$I_n(x) = (-i)^n J_n(ix) \quad (4-13)$$

$$\begin{aligned} K_n(x) &= \frac{\pi}{2} i^{n+1} H_n^{(1)}(ix) \\ &= \frac{\pi}{2} i^{-n-1} H_n^{(2)}(-ix) \\ &= -\frac{\pi}{2} \operatorname{Re} [i^n N_n(ix)] \end{aligned} \quad (4-14)$$

Asymptotic Expansions

For large argument, x , the functions $I_p(x)$ and $K_p(x)$ may be expressed asymptotically in terms of the convergently beginning series:

$$\begin{aligned} \bar{C}(s) &= 1 + \frac{1}{8} \left(\frac{1}{s} - \frac{5p^2}{3s^3} \right) \\ &+ \frac{1 \cdot 3}{8^2} \left(\frac{3}{2s^2} - \frac{77p^2}{9s^4} + \frac{385p^4}{54s^6} \right) \\ &+ \frac{1 \cdot 3 \cdot 5}{8^3} \left(\frac{5}{2s^3} - \frac{1521p^2}{50s^5} + \frac{17017p^4}{270s^7} - \frac{17017p^6}{486s^9} \right) + \dots \end{aligned} \quad (4-15)$$

The series must be stopped when the terms no longer decrease.

If the m 'th term is written in the form:

$$\frac{(2m-1)(2m-3)\dots 1}{(8s)^m} \sum_{n=0}^m C_{m,n} (-1)^n (p/s)^{2n}$$

the coefficients $C_{m,n}$ are given by the relations:

$$C_{m+1,n+1} = \frac{2k+1}{(2m+1)(k+1)} [(2k-3)C_{m,n} + (2k+1)C_{m,n+1}] \quad (4-16)$$

$$k = m + 2n + 2$$

$$C_{0,0} = 1$$

$$C_{m,-1} = C_{m,m+1} = 0$$

The functions $I_p(x)$ and $K_p(x)$ of large argument can then be represented asymptotically as follows:*

$$I_p(x) \sim \frac{1}{\sqrt{2\pi s}} \left(\frac{s-p}{s+p}\right)^{p/2} e^s \bar{C}(s) \quad (4-17)$$

$$K_p(x) \sim \sqrt{\frac{\pi}{2s}} \left(\frac{s+p}{s-p}\right)^{p/2} e^{-s} \bar{C}(-s) \quad (4-18)$$

$$\text{where: } s = \sqrt{x^2 + p^2}$$

As x becomes large:

$$s \sim x$$

$$\bar{C}(s) \rightarrow 1$$

$$\bar{C}(-s) \rightarrow 1$$

* See Reference 22, Chapter 8.

Limiting Cases of the Moving Source Solutions

The expansions (4-6) and (4-8) are sufficient to evaluate expression (3-50). It is desired to find :

$$\lim_{r \rightarrow 0} F(r)$$

$$F(r) = r^2 \left[I_0(2Vr) K_0(Vr) + I_1(2Vr) K_1(2Vr) \right]$$

Neglecting higher order terms, this function can be written as follows, by use of (4-6) and (4-8):

$$F(r) \sim r^2 \left[-\ln(Vr) + Vr(\ln Vr + \frac{1}{2Vr}) \right]$$

Noting that:

$$\lim_{r \rightarrow 0} [r \ln(Vr)] = \lim_{r \rightarrow 0} \ln(Vr^F r^F) = \ln 1 = 0$$

it is easily seen that:

$$\lim_{r \rightarrow 0} F(r) = 0$$

Source of High Velocity

Consider first the case of the moving point source. The temperature U is given by equation (3-26), which is repeated here:

$$U_p = \frac{2P}{\pi} e^{-2VZ} K_0(2VR) \quad (4-19)$$

If the temperature is observed at a point on the stationary X-Y plane as a function of time for large velocity, it might be expected that, in the limit, the temperature would be described by the one-dimension source function (3-12). The source moves past the vicinity of the point of observation in a very short time, depositing a certain amount of heat on the line of its path. By the time this heat has diffused appreciably away from the line, the source is far away, and has little effect on the temperature at the point of observation. The case is similar to the case where a quantity of heat, uniformly distributed along a straight line, is suddenly released on the plane, a situation where (3-12) applies, and it will be shown here that in the limit of large velocity, (4-19) does, in fact, reduce to (3-12).

First, it is convenient to adjust P_p , the rate of heat emission from the source, such that one unit of heat is emitted per unit distance travelled:

$$P_p = V \quad (4-20)$$

Z and R can be expressed in terms of time W from equations (3-27) and (3-28). Setting X equal to zero, it is found that W is the elapsed time between: a) the time of closest approach of the source to the point of observation, and b) the time of observation. Y, then, becomes the distance from the path of the source to the point of observation. Making these substitutions in (4-19):

$$U_p = \frac{2V}{\pi} e^{2V^2W} K_0 [2V \sqrt{Y^2 + V^2W^2}] \quad (4-21)$$

The radical in (4-21) can be expanded by the binomial theorem:

$$\sqrt{V^2W^2 + Y^2} = VW + \frac{Y^2}{2VW} + \dots \quad (4-22)$$

As V becomes large, higher order terms may be neglected. Also, from (4-18), it is seen that, for large V ;

$$K_0(2VR) \sim \sqrt{\frac{\pi}{4VR}} e^{-2VR} \quad (4-23)$$

Substituting (4-22) and (4-23) into (4-21):

$$U_p \sim \frac{2V}{\pi} e^{2V^2W} \sqrt{\frac{\pi}{4V^2W + 2Y^2/W + \dots}} e^{-2V^2W - Y^2/W - \dots}$$

Simplifying, and neglecting higher order terms, it is found that:

$$U_p \sim \frac{1}{\sqrt{\pi W}} e^{-Y^2/W} \quad (4-24)$$

Which is, indeed, of the same form as (3-12).

Consider now the temperature at the center of a moving uniform circular source as the velocity becomes large. The temperature is given by (3-41) for a source of unit radius:

$$U_c = 2 P_c [I_0(2V) K_0(2V) + I_1(2V) K_1(2V)] \quad (4-25)$$

If the center of the source passes over a point on the stationary X-Y plane at sufficiently large velocity, there will be negligible conduction away from the point while the source is in the same vicinity. The amount of heat at the point when the center of the source coincides with the point will be the amount of heat deposited by the part of the source which has already passed over the point. Since the radius of the source is unity, heat will have been deposited at the rate P_c for a length of time $1/V$. The temperature will therefore be:

$$U_c \sim \frac{P_c}{V} \quad (4-26)$$

It will be shown that (4-25) does indeed approach (4-26) in the limit of large velocity.

From (4-17) and (4-18) it is seen that, as V becomes large:

$$I_p(2V) K_p(2V) \sim \frac{1}{4V} \quad (4-27)$$

Substitution of (4-27) into (4-25) gives:

$$U_c \sim \frac{P_c}{V}$$

which agrees with (4-26).

Small Velocity, Moving Point Source

If the velocity is now permitted to approach zero, it becomes apparent that the solution for the moving point source should approach the steady state solution of a stationary point source emitting heat continuously. Solving first the steady state problem, it is seen that the temperature is a function of R only, where R is the distance from the source. Expressed in terms of the real rate of heat emission p_p , the temperature is governed by the differential equation:

$$p_p = -2\pi R k \frac{dU}{dR} \quad (4-28)$$

where p_p is the rate of heat flow across a cylindrical surface of radius R , whose axis passes through the source. The normalized rate of heat flow, P_p , is given by (3-30):

$$P_p = \frac{1}{4k} p_p$$

so that:

$$P_p = -\frac{\pi}{2} R \frac{dU}{dR} \quad (4-29)$$

Equation (4-29) may be solved by the usual methods to give the difference in temperature between two values of R:

$$U_a - U_b = \frac{2P}{\pi} \ln(b/a) \quad (4-30)$$

where U_a = temperature at $R = a$
 U_b = temperature at $R = b$

Consider now the case of the moving point source, which gives solution (4-19). The difference between the temperatures at $R = a$ and $R = b$ is found to be:

$$U_{pa} - U_{pb} = \frac{2P}{\pi} [e^{-2VZ_b} K_0(2Vb) - e^{-2VZ_a} K_0(2Va)] \quad (4-31)$$

As V becomes small, the exponentials approach unity, and from (4-8):

$$K_0(2VR) \sim -\ln(VR) \quad (4-32)$$

Equation (4-31) can then be represented as:

$$U_{pa} - U_{pb} \sim \frac{2P}{\pi} [\ln(Vb) - \ln(Va)] = \frac{2P}{\pi} \ln(b/a) \quad (4-33)$$

which agrees with (4-30).

CHAPTER IV

V. Mathematical Analysis for Computer Programming

The temperature on a plane at point (A, B) due to a uniform circular source moving at constant velocity V may be found by evaluating expression (3-35). This expression involves a surface integral, which may be expressed as an equivalent double integral over the two variables Z_1 and Y_1 . Unfortunately, no method was found of performing this integration by analytical techniques, so it became necessary to use numerical methods.

Although double integration by numerical methods presents no basic difficulties other than those found in integration over a single variable, the actual procedure becomes much more tedious because of the many points at which the integrand must be evaluated. The task is further complicated in the problem considered here in that the double integral is a function of three parameters: A, B, and V. If it is desired to compute tables of the values of the integral for, say, twenty values of each parameter, in all combinations, the integration would have to be carried out 8000 times, a considerable task even for a modern large scale digital computer. It therefore becomes expedient to find a method of numerical integration which requires that the integrand be evaluated at a comparatively small number of points, while giving a result of sufficient accuracy.

A convenient specification of the accuracy of a method of numerical integration is its "degree of precision." Suppose that the expression:

$$\int_a^b w(x) f(x) dx \quad (5-1)$$

is to be evaluated by numerical methods, where $w(x)$ is some weighting function. If the numerical method gives an exact result when $f(x)$ is any arbitrary polynomial of degree r or less, but fails to give an exact result for at least one polynomial of degree $r+1$, the method is said to have degree of precision r .

Suppose now that $f(x)$ is an arbitrary function. Integral (5-1) may be evaluated approximately by evaluating $f(x)$ at n values of x , finding a polynomial which passes through these points, and computing the integral of the polynomial. Since n points determine a polynomial of degree $n-1$, it would be expected that a formula for numerical integration could be derived which has degree of precision $n-1$, and this is indeed the case. Such a formula can be expressed in the form:

$$\int_a^b w(x) f(x) dx \approx \sum_{i=1}^n h_i f(x_i) \quad (5-2)$$

where the h_i are determined by the x_i 's and the weighting function $w(x)$.

Now suppose that both $f(x)$ and $f'(x)$ -- the derivative of $f(x)$ -- are specified at the n points x_1, x_2, \dots, x_n . These data are sufficient to determine uniquely a polynomial of degree $2n-1$ which has the same ordinate and slope as the function $f(x)$ at each of the points x_i . Integral (5-1) may then be approximated by a formula of the form:

$$\int_a^b w(x) f(x) dx \approx \sum_{i=1}^n h_i f(x_i) + \sum_{i=1}^n \bar{h}_i f'(x_i) \quad (5-3)$$

which has degree of precision $2n-1$.

It turns out that for many weighting functions $w(x)$, and suitable limits a and b , that the points x_i may be chosen such that all of the coefficients \bar{h}_i become zero, so that (5-3) becomes independent of $f'(x_i)$. This leads to the remarkable result that a degree of precision $2n-1$ may be attained in numerical integration in a process which requires the evaluation of $f(x)$ at only n points! Numerical integration of this type is known as Gaussian quadrature.

Two weighting functions, $w(x)$, are of particular interest here, namely:

$$w(x) \equiv 1 \quad (5-4)$$

and

$$w(x) = \sqrt{1 - x^2} \quad (5-5)$$

$$a = -1, \quad b = 1$$

In the first case, where $w(x)$ is identically equal to one, it is convenient to set the limits of integration, a and b , to -1 and $+1$, respectively. Any definite integral of the form (5-1) can be expressed as an integral between limits -1 and $+1$ by a suitable change in the variable of integration.

Formula (5-3) becomes:

$$\int_{-1}^1 f(x) dx \approx \sum_{i=1}^n h_i f(x_i) \quad (5-6)$$

The point x_i is then prescribed to be the i -th zero of the n -th Legendre polynomial, $P_n(x)$. The coefficients h_i become:

$$h_i = \frac{2(1-x_i^2)}{(n+1)^2 [P_{n+1}(x_i)]^2} \quad (5-7)$$

In the second case, where the weighting function and limits of integration are given by equations (5-5), the integration formula may be expressed as follows:

$$\int_{-1}^1 \sqrt{1-x^2} f(x) dx \approx \sum_{i=1}^n \lambda_i f(x_i) \quad (5-8)$$

The points x_i and the coefficients λ_i are, in this case, associated with the Tchebicheff polynomials of the second kind; they may be expressed in terms of trigonometric functions as:

$$x_i = -\cos \frac{i}{n+1} \pi \quad (5-9)$$

$$\lambda_i = \frac{\pi}{n+1} \sin^2 \frac{i}{n+1} \pi \quad (5-10)$$

$$i = 1, 2, 3, \dots, n-1, n$$

These two cases, where $w(x)$ is equal to unity, and where $w(x)$ is equal to $\sqrt{1-x^2}$ are known as Legendre-Gauss quadrature and Tchebichef-Gauss quadrature, respectively. If n is the number of the points x_i , both of the formulas (5-6) and (5-8) have degree of precision $2n-1$, provided the points x_i are chosen as directed. A development of these ideas will be found in Reference 13, Chapter 10. A large amount of useful information on orthogonal polynomials, which are involved in the derivation of Gaussian quadrature formulas, appears in Reference 17, Chapter 10.

Numerical integration by Gaussian quadrature must be used with discretion, for there are cases where other integration procedures are to be preferred. If the function $f(x)$ has a singularity in, or near, the interval of integration, Gaussian quadrature may lead to results of very poor accuracy. If the number of points, n , is increased, the accuracy of the result may very well decrease, a situation being reached where the results from Gaussian quadrature oscillate with increasing amplitude about the true value of the integral, as the number of points is increased. In such cases, integration by the trapezoid rule, or by Simpson's rule, may be appropriate.

In evaluating integral (3-35), three different cases are considered, depending on the location of the point of observation (A, B) in relation to the source.

Case I, $\sqrt{A^2 + B^2} > 2$

In this case, the point of observation is far enough from the source so that the singularity of the integrand at ($A = Y_1, B = Z_1$) is not expected to cause difficulty in integration by Gaussian quadrature. Equation (3-35) is expressed in the form (3-36). It will be seen that the outer integral of (3-36) is of the same form as (5-7), so that integration may be done by Tchebichef-Gauss quadrature. The inner integral of (3-36) is evaluated by Legendre-Gauss quadrature.

Case II, $1.05 < \sqrt{A^2 + B^2} < 2$

In this case, the singularity is near the region of integration. The integration is done according to equation (3-36), but the inner integral is evaluated by Simpson's rule, while Tchebichef-Gauss quadrature is used to evaluate the outer integral.

Case III, $\sqrt{A^2 + B^2} < 0.95$

In this case, the singularity is within the region of integration, so that special techniques must be used to obtain accurate results.

The integration in (3-35) is to be carried out over the interior of a unit circle whose center is at the origin of the $X_1 - Y_1$ plane. It is convenient to separate this region into two parts, and carry out the integration in each part separately. Consider first the region on the interior of a circle whose center is at (A, B) , and which is tangent to the unit circle, as shown in Figure 2. The integral over this region is given by (3-50), where F_r is given by

$$F_r = 1 - \sqrt{A^2 + B^2} \quad (5-9)$$

The integral over the remaining area inside the unit circle may be expressed as:

$$\frac{2}{\pi} P_c \int_{1 - \sqrt{A^2 + B^2}}^{1 + \sqrt{A^2 + B^2}} R_1 K_0(2VR_1) \int_{\alpha_1(R_1)}^{\alpha_2(R_1)} e^{2VR_1 \cos \theta} d\theta dR_1 \quad (5-10)$$

where:

$$R_1 = \sqrt{(A - Z_1)^2 + (B - Y_1)^2}$$

$$\alpha_1(R_1) = \theta + |\beta_1|$$

$$\alpha_2(R_1) = \theta + 2\pi - |\beta_1|$$

$$\cos \beta_1 = \frac{1 - \sqrt{A^2 + B^2} - R_1^2}{2 R_1 \sqrt{A^2 + B^2}}$$

$$\phi = \cos^{-1} \frac{A}{\sqrt{A^2 + B^2}}$$

Integral (3-35), then, is equivalent to the sum of (5-12) and (3-50), with F_r given by (5-9). Evaluation of the inner integral of (5-12) is done by Legendre-Gauss quadrature; the outer integral is evaluated by Simpson's rule.

Finally, in the region $0.95 \sqrt{A^2 + B^2} < 1.05$, the integration is not to be carried out at all, since it would be necessary to compute the integrand at a large number of points to obtain accurate results, due to the close proximity of the singularity to the region of integration.

CHAPTER VI

VI. Programming Techniques

General

An IBM 704 computer program entitled HOT SPOT has been written to evaluate the temperature on a plane containing the uniform circular heat source in uniform rectilinear motion

The IBM 704 computer at the Massachusetts Institute of Technology is a large-scale digital computer with a full complement of peripheral equipment. It has 32,768 registers of random access magnetic core storage, each register providing storage for 36 bits of binary information. In view of the large storage capacity, the general philosophy of programming this problem has been to consider speed of execution to be of primary importance, with only secondary regard for minimizing the storage space required for the program.

For purposes of discussion, the program may be conveniently divided into sections as follows:

- A. Initialization
- B. Administration of computation
- C. Report of results
- D. Subroutines for evaluation of integrands
- E. Integration subroutines
- F. Subroutines for evaluation of modified Bessel functions
- G. Subroutines for evaluation of other functions
- H. Post-Mortem and Printing routines

Sections A, B, and C.

The flow diagram through Sections A, B, and C is shown in Figure 3. Section A includes the blocks labelled "Initialize" and "PVR1". The "Initialize" block places initial quantities in certain of the storage registers, e.g., it places zero in the register containing the run number. PVR1 is a parameter variation routine, which selects values for A, B, and V from tables stored in the computer memory. It is a closed subroutine whose calling sequence is:

```

L      TSX   PVR1, 4
L + 1  PZE   P1, 0, N1
L + 2  PZE   P2, 0, N1
L + 3  PZE   P3, 0, N3
L + 4  (RETURN AFTER ALL VARIATIONS HAVE BEEN MADE)
L + 5  (RETURN AFTER EACH VARIATION)

```

P1, P2, and P3 are the addresses of the tables from which the parameter values are to be selected; N1, N2, and N3 are the numbers of values to be chosen from each table. Each quantity in the tables is considered by the routine to occupy two registers of storage, so that if only one register is needed, as is true in this program, the successive values in tables P1, P2, and P3 should be placed in every second register. For example, if the first three values to be used for the parameter which is listed in table P1 are to be 1.0, 2.0, and 3.0, the table would appear as follows.

```

P1  DEC 1.0
    PZE 0
    DEC 2.0
    PZE 0
    DEC 3.0
    PZE 0

```

...

As the routine is entered repeatedly, it picks up succeeding values in each table and stores them in locations A, B, and V respectively, in such a way that all combinations of the values for the three parameters are eventually chosen. If, for example, the first three values in tables P1, P2, and P3 were (1, 2, 3), (4, 5, 6), and (7, 8, 9), respectively, the contents of registers A, B, and V after successive entries to the routine would be:

	C(A)	C(B)	C(V)
after 1st entry	1	4	7
after 2nd entry	2	4	7
after 3rd entry	3	4	7
after 4th entry	1	5	7
after 5th entry	2	5	7
· · ·	·	·	·
after 26th entry	2	6	9
after 27th entry	3	6	9

After values have been selected for A, B, and V, the evaluation of the double integral is done. The type of integration and the number of points to be used is first decided on the basis of the magnitude of $\sqrt{A^2 + B^2}$ (See Chapter 5), and control is transferred to the pertinent computation routine, which performs the evaluation of the double integral. The results of the computation and certain statistics are stored in core memory to be printed and/or punched out at the end of the run. Storage space is provided for 1000 computations. If desired, the results of the evaluations of the inner integral, along with certain other intermediate results, may be printed out by placing sense switch 2 in down position. This is not recommended for long runs however, because of the large amount of printed material which will be produced.

After the results of the computation are stored, control is normally transferred back to PVR1, which selects another combination of parametric values, and proceeds as before. Provision has been made, however, to print out the results and terminate the computer run at any time, by placing switch 6 in "down" position.

The results and statistics of the run are printed in separate tables. The table of results lists the values of A, B, V, the result for $U(A, B)$ —the temperature at point (A, B) from a source of unit radius moving at velocity V, emitting normalized heat at a total rate (not density rate) of unity. For purposes of comparing curve shapes for different values of V, the ratio of $U(A, B)/U(0, 0)$ is also listed under "Normalized U".

A table of statistics is printed which lists the region in which the point is located (region 1—inside source, region 2—outside source), the number of points used in the evaluation of the outer integral, the minimum and maximum number of points used in evaluation of the inner integral, and the factor— $U(0, 0)$ —used in computing the "Normalized U."

Sections D and E

The subroutines for evaluating the integrals are all quite similar in their flow diagrams, so only the diagram for the routine used in Case III ($\sqrt{A^2 + B^2} < 0.95$) is shown here as an example. (Figure 4)

The integration subroutines themselves first assign a value to the variable of integration, then refer repeatedly to a satellite subroutine to evaluate the integrand at the assigned points, multiply these evaluations by the appropriate factors, and perform the summation. In case III, the integration routines also compute the limits of integration, although this is unnecessary in cases I and II, since the limits are always -1 and 1.

The values of the independent variable are assigned by the integration formula in the Gaussian quadrature integrations. In the case of Simpson's rule, however, arbitrary points may be chosen. In this program, the spacing of points for Simpson's rule is determined such that the area under the curve of the integrand between two adjacent points x_1 is

approximately the same for all pairs of adjacent points. This is accomplished, in the program, by evaluating the integrand at the beginning of the interval of integration, and setting the distance to the next point to be evaluated, equal to a constant divided by the integrand at the first point. This procedure is repeated until the end of the interval is reached. The constant is computed from a first approximation of the integral by an evaluation using five equally spaced points, and from information supplied previously as to the number of points to be used. The approximate number of points to be used must be stored in location PARN before the routine is entered. The actual number of points will appear in location PARN+1 upon exit from the routine.

The subroutine for performing integration by Simpson's rule has the following calling sequence:

```

L      TSX  SIMR1, 4
L + 1  NOP
L + 2  (NORMAL RETURN)

```

The routine is to be entered with the lower limit of integration in the AC, the upper limit in the MQ. A satellite subroutine for evaluation of the integrand must be in core storage, and must have the calling sequence:

```

      TSX  FOFX, 4
      (ERROR RETURN)
      (NORMAL RETURN)

```

The integration routine SIMR1 first assigns values to the variable of integration, evaluates the integrand at these points, and stores these data in tables in core storage. The integration is done by the SHARE subroutine UA CLINT4.

The number of points for the Gaussian quadrature subroutines is specified in the calling sequence. There are three such subroutines in this program, with calling sequences as follows

TSX GQI, 4	TSX HQI, 4	TSX GQT, 4
PZE N, 0, 1	PZE N, 0, 1	PZE N
(NORMAL RETURN)	(NORMAL RETURN)	(NORMAL RETURN)

N is the number of points to be used in evaluating the integral. The respective satellite subroutines must have the following calling sequences

TSX FOFX, 4	TSX HOFX, 4	TSX FOFY, 4
(ERROR RETURN)	(ERROR RETURN)	(ERROR RETURN)
(NORMAL RETURN)	(NORMAL RETURN)	(NORMAL RETURN)

The subroutine GQI is a relativized SHARE subroutine (BS GQI). Subroutine HQI is identical to GQI except that the symbols have been changed to permit both routines to be used concurrently. These routines will perform Legendre-Gauss quadrature integration between arbitrary limits. Upon entry to the subroutines, the AC must contain the lower limit, the MQ must contain the upper limit, upon exit from the routine, the AC contains the value of the integral.

Subroutine GQT is a Tchebichef-Gauss quadrature routine, written especially for this program. (See Chapter 5, equations 5-8, 5-9, and 5-10). The number of points, N, must be one of the following: 1, 2, 3, 4, 5, 8, 11, 14, 17, 29, or 35. If N, as specified in the calling sequence (see above), is not equal to one of these, an error stop will result. The routine contains tables of x_i and $(N+1)\lambda_i$ (see Chapter 5) for $N=29$ and for $N=35$. If it is desired to use a number of points n which is not equal to 29, or 35, the x_i and λ_i may be found from the tables as shown in the following example.

Suppose it is desired to use 4 points in evaluating the integral. Reference to equation (5-9) shows that the x_i may be found by taking every sixth value from the table of x_i 's for $N=29$. The values of x_1 , x_2 , x_3 , and x_4 would be the 6th, 12th, 18th and 24th values in the x_i table for $N=29$. Similarly, equation (5-10) shows that the coefficient λ_i for $n=4$ may be found by selecting $(N+1)\lambda_i$, and dividing these values by $n+1$ ($=5$). The procedure may be simplified by performing the division after the sum has been taken (equation 5-8), so that only one division need be performed.

The satellite subroutines for evaluation of the integrands perform straightforward computation as indicated by the pertinent equation, as explained in Chapter 5. The same subroutines are used in Cases I and II, where $\sqrt{A^2 + B^2} > 1.05$, and have the calling symbols FOFY for the outer integrand, and FOFX for the inner integrand. In Case III, where $\sqrt{A^2 + B^2} < 0.95$, the subroutines which evaluate the outer and inner integrand have the calling symbols FOFXB, and HOFX, respectively. The integration routine SIMRI is used in both Cases II, and III, and refers to FOFX for evaluating the integrand, so that some means must be provided to distinguish between the two cases when the integrand is evaluated. The program does this by placing the instruction NOP in location FOFX during computation in Case II, and by placing the instruction TRA FOFXB in location FOFX in Case III.

Section F

It was found necessary to write subroutines for the evaluation of the modified Bessel functions $I_0(x)$, $I_1(x)$, $K_0(x)$, and $K_1(x)$. In view of the similarities in the expansion of some of these functions, these subroutines were incorporated into a single package.

For an argument which is not too large, the functions $I_0(x)$ and $I_1(x)$ are conveniently expanded as infinite series; the functions $K_0(x)$ and $K_1(x)$ may be expanded in terms of a known function plus an infinite series, as explained in Chapter 4. For large argument, ($x > 9.9$) the number of terms which must be taken to obtain results of sufficient accuracy becomes excessive, so that it is preferable to use asymptotic expansions. Computation of the functions $K_0(x)$ and $K_1(x)$ for arguments between $x=2$ and $x=10$ becomes

complicated by the behavior of the terms in the series expansion (4-8). As x becomes larger, the infinite series, and the term containing the logarithm both become large in magnitude, but their sum becomes quite small, so that it becomes necessary to use double precision programming to attain sufficient accuracy. Since double precision arithmetic takes considerable computer time, it was decided to use a table look-up and interpolation procedure to find $K_0(x)$ and $K_1(x)$ when $2.0 < x < 9.9$. The SHARE subroutine WK LIN1 is used for this purpose. This subroutine is entered with x on the AC, it then locates the three best table values, and applies a three-point Lagrangian interpolation formula to find the value of $K_0(x)$ or $K_1(x)$.

The modified Bessel function package also contains subroutines for the evaluation of the products $I_0(x)K_0(x)$, and $I_1(x)K_1(x)$, and products of exponential functions by modified Bessel functions. Although these subroutines are not particularly useful normally, they permit computations to be made for larger arguments than would otherwise be possible. Consider, for example, the function:

$$e^y K_0(x)$$

where x and y are positive and almost equal. If the exponential and the modified Bessel function are computed separately and multiplied, it will be found that if their arguments are greater than approximately 67, computer overflow will result in the case of the exponential, and underflow will result in the case of the Bessel function. If, however, $K_0(x)$ is expanded asymptotically by (4-18), and the arguments of the exponentials combined before the function is evaluated, the computation can be carried out for arguments up to about 10^{38} !

It is found that the infinite series expansions for the modified Bessel functions may all be expressed in the following form:

$$Z(x) = G(x) + H(x) [C_0 + C_1 F(x) + C_2 F^2(x) + \dots]$$

If $Z(x)$ equals $K_1(x)$, for example, reference to (4-8) shows that:

$$F(x) = \left(\frac{x}{2}\right)^2$$

$$G(x) = I_1(x) \ln \left(\frac{x}{2}\right) + \frac{1}{x}$$

$$H(x) = \frac{x}{2}$$

The constants C_0, C_1, \dots , depend upon the particular function to be expanded. The series expansions in the modified Bessel function package are evaluated by a satellite subroutine which was incorporated within the package, and which evaluates the series when given $F(x)$, $G(x)$, and $H(x)$, and the address of a table containing C_0, C_1 , etc. In order to attain maximum speed of computation, tables of the constants C_0, C_1, C_2, \dots , are stored in core memory, as well as tables from which may be determined the number of terms to be computed in the series. If the number of terms in the series is known, the computation may be performed by expressing the series in the form:

$$C_0 + x[C_1 + x(C_2 + \dots)]$$

and performing the computation by the loop:

```

LXA  N, 1
LDQ  C,-1, 1
TRA  *+2
LDQ  SUM
FMP  X
FAD  C, 1, 1
STO  SUM
TIX  *-4, 1, 1
FAD  C

```

where N contains the power of the highest order term.
 Each coefficient C_n is stored in location $C - n - 1$.

It will be noted that only one multiplication and one addition are necessary for each additional term in the series.

If, on the other hand, the number of terms is not known, each term must be computed separately, requiring two multiplications, and compared with the cumulative sum to determine when an adequate number of terms have been taken. Since each floating point multiplication takes twenty cycles of computer time (compared with two cycles for most comparing, storage, and transfer operations), this method requires considerably more computer time than the first method.

The number of terms required is determined, by a satellite subroutine, from a table which lists the arguments of the series in the order of the number of terms required. The maximum argument for which terms may be used appears in location $L-n$, the maximum number of terms which may be used in any series appears in the address part of location $L + 1$. The subroutine is entered with the argument of the series in the AC. The routine then searches the table of arguments, indexing on I. R. 2, until it finds the number of terms needed, then leaves the subroutine with the power of the highest order term in I. R. 2. The subroutine which evaluates the series may then be entered directly.

The calling sequences for the modified Bessel functions are identical except for the calling symbol:

TSX SYMBOL; 4
 (NORMAL RETURN)

SYMBOL	FUNCTION COMPUTED
BSI0	$I_0(x)$
BSI1	$I_1(x)$
BSK0	$K_0(x)$
BSK1	$K_1(x)$
BSP0	$I_0(x) K_0(x)$
BSP1	$I_1(x) K_1(x)$
BXI0	$e^y I_0(x)$
BXI1	$e^y I_1(x)$
BXK0	$e^y K_0(x)$
BXK1	$e^y K_1(x)$

The subroutines are entered with x in AC, and (where applicable) y in the MQ; upon return, the function appears in the AC. For example, if the contents of ARG is x , the sequence:

```

CLA  ARG
TSX  BSI0, 4
STO  Z

```

will place $I_0(x)$ in location Z.

Sections G and H

The binary decks MI-PMPK and REAL-FUNCTIONS-PACKAGE must be read into core memory before computation can begin. REAL-FUNCTIONS-PACKAGE contains subroutines for evaluation of various functions, of real argument, such as the exponentials, sine, cosine, square root, etc. MI-PMPK contains various output, error checking, and post-mortem routines.

Error Detection and Post Mortems

Virtually all floating point addition, subtraction, multiplication and division instructions are followed by one of the instructions:

TSX ASMOV, 4

TSX DIVOV, 4

These subroutines check the status of the overflow and divide check indicators to determine whether overflow or underflow has occurred, or whether an illegal division (such as division by zero) has been attempted. In case of underflow, control is returned to the program with the result of the attempted operation set to zero. An overflow or attempt at illegal division results in a transfer of control to the post-mortem program, which prints out the machine conditions and the location of the TSX ASMOV or TSX DIVOV instruction which led to the post-mortem. Control is then transferred to location HSPPM, which prints out the contents of certain regions of core memory, to facilitate diagnosis of the error. After the first three error stops, control is transferred to location START, from which the program proceeds with the next computation. After the fourth error stop, however, control is transferred to REPORT, resulting in the print-out of results and termination of the run.

Instructions for use of the Program

- 1) Place the values to be used for A in locations TABLA, TABLA+2, TABLA+4, etc. (Space reserved for 31 values).
- 2) Place the values to be used for B in TABLB, TABLB+2, etc. (Space reserved for 22 values).
- 3) Place the values to be used for V in TABLV, TABLV+2, etc. (Space reserved for 25 values).
- 4) Place the following pseudoinstructions in the indicated locations in the program deck.

START+7	PZE	TABLA, 0, N1
START+8	PZE	TABL B, 0, N2
START+9	PZE	TABL V, 0, N3

N1, N2, N3 are the number of values of the respective parameters to be used. Caution: the number of combinations equals $N1 \times N2 \times N3$.

CHAPTER VII

VII. Summary and Conclusions

Use of the Computer Program

The computer program, which was discussed in the last chapter, evaluates the temperature rise, $U_t(A, B, V, P_t)$, at point (A, B) on a flat infinite, perfectly insulated plate, if there is a uniform circular source of heat moving in a straight line on the plate at a constant normalized velocity, V . The source is of unit radius, and emits one unit of normalized heat per unit normalized time, i. e. P_t is equal to unity. In order to make practical use of these solutions, it is necessary to relate the normalized rate of heat flow, P_t , and the normalized velocity, V , to the real physical quantities; this is done by the expressions following equation (3-57). If the radius of the source is equal to some number F , rather than unity, the temperature rise on the plate is given in terms of the temperature rise from a source of unit radius by equation (3-59).

The use of the program in the electron beam etching problem, discussed in Chapters I and II, is expected to be along the following lines. First it will be necessary to decide, from the nature of the film, the temperature rise necessary to produce a sufficient rate of sublimation or evaporation, and the degree to which the temperature rise must be confined within the vicinity of the scanning electron beam in order that sublimation or evaporation occur only at the desired locations. The computer program may then be used to find an estimate of the scanning velocity and rate of heat flow required.

a trial and error method will have to be used in making these computations on the computer, where calculations are made for several different velocities to find the velocity which gives the required temperature distribution. It would be advisable to make initial computer runs to calculate tables of the temperature distributions at several velocities,

so that a first estimate of the velocity required may be found in any particular problem, as a guide to the selection of velocities for further computations. Such tables need not be extensive at first, but should be expanded as more calculations are made from time to time.

If the maximum temperature rise for a given velocity, source radius, and rate of heat input, is desired, a fairly good approximation may be found by calculating the temperature at the point (0, 0) from equations (3-57) and (3-59). The asymptotic behavior of the temperature distribution for small and large velocities would lead one to expect that the maximum temperature on the plane would be somewhere between the temperature at the point (0, 0) and twice the temperature at the point (0, 0).

Suggestions for Further Work on the Computer Program

As the program now stands, the number of points used in the evaluation of the inner integrals is equal to the number of points used in evaluating the outer integral, as determined in Section B of the program. It would be advantageous to find a way to modify the program so that, in a single evaluation of the outer integral, the number of points in the inner integral is varied such that those integrals which make a large contribution to the result are evaluated by use of many points, while those making a small contribution are evaluated by taking few points. The time required for computation could probably be reduced by a factor of one-third by such a modification.

The number of points to be used in evaluation of the integrals is determined by the contents of the blocks of ten registers of core storage preceding each of the symbols HANO, HBNO, HCNO. (See program listing) It may be advisable to perform some experimentation to determine the optimum figures for most efficient

computation. An error analysis of the numerical integration techniques would be most helpful in deciding the number of points to be used.

If extensive use is to be made of the program, it is strongly suggested that some sort of error evaluation be made. This can probably be most easily done by making calculations for a few sample combinations of parametric values. Two calculations could be made for each combination, using different numbers of points in the numerical integrations. Comparison of the results should provide a reasonably good criterion for estimating the accuracy.

Concluding Remarks

The material presented here, and the I. B. M. 704 computer program, should provide a basis for further study of the electron beam etching problem. Care should be exercised in the use of the computer results, however, so that they are not applied outside of the regions where they are valid, as discussed in Chapter II. If such precautions are observed, however, it is expected that this work will provide a better understanding of the potentialities and limitations of the production of micro-miniature components and circuits by electron beam etching.

List of Symbols

U = temperature

U_p = temperature due to a point source in uniform rectilinear motion

U_c = temperature due to a uniform circular source of unit radius
in uniform rectilinear motion, in terms of the rate of heat
flow per unit area of the source

U_t = temperature due to a uniform circular source in uniform recti-
linear motion, in terms of the rate of total heat flow from
the source

U'_c = temperature due to a moving circular source of radius F ,
in terms of the rate of heat flow per unit source area

U'_t = temperature due to a moving circular source of radius F ,
in terms of the rate of total heat flow from the source

t = real time

T = normalized time

q = real quantity of heat

Q = normalized quantity of heat

v = real velocity

V = normalized velocity

p = real rate of real heat flow

P = normalized rate of normalized heat flow

k' = bulk thermal conductivity

ρ' = volume density

C' = volume thermal capacity

k = two-dimensional thermal conductivity of a plate

ρ = area density of a plate

C = area thermal capacity of a plate

d = plate thickness

a'^2 = bulk thermal diffusivity

a^2 = two-dimensional thermal diffusivity of a plate

$I_n(x)$ = the modified Bessel function of the first kind, order n

$K_n(x)$ = the modified Hankel function of order n

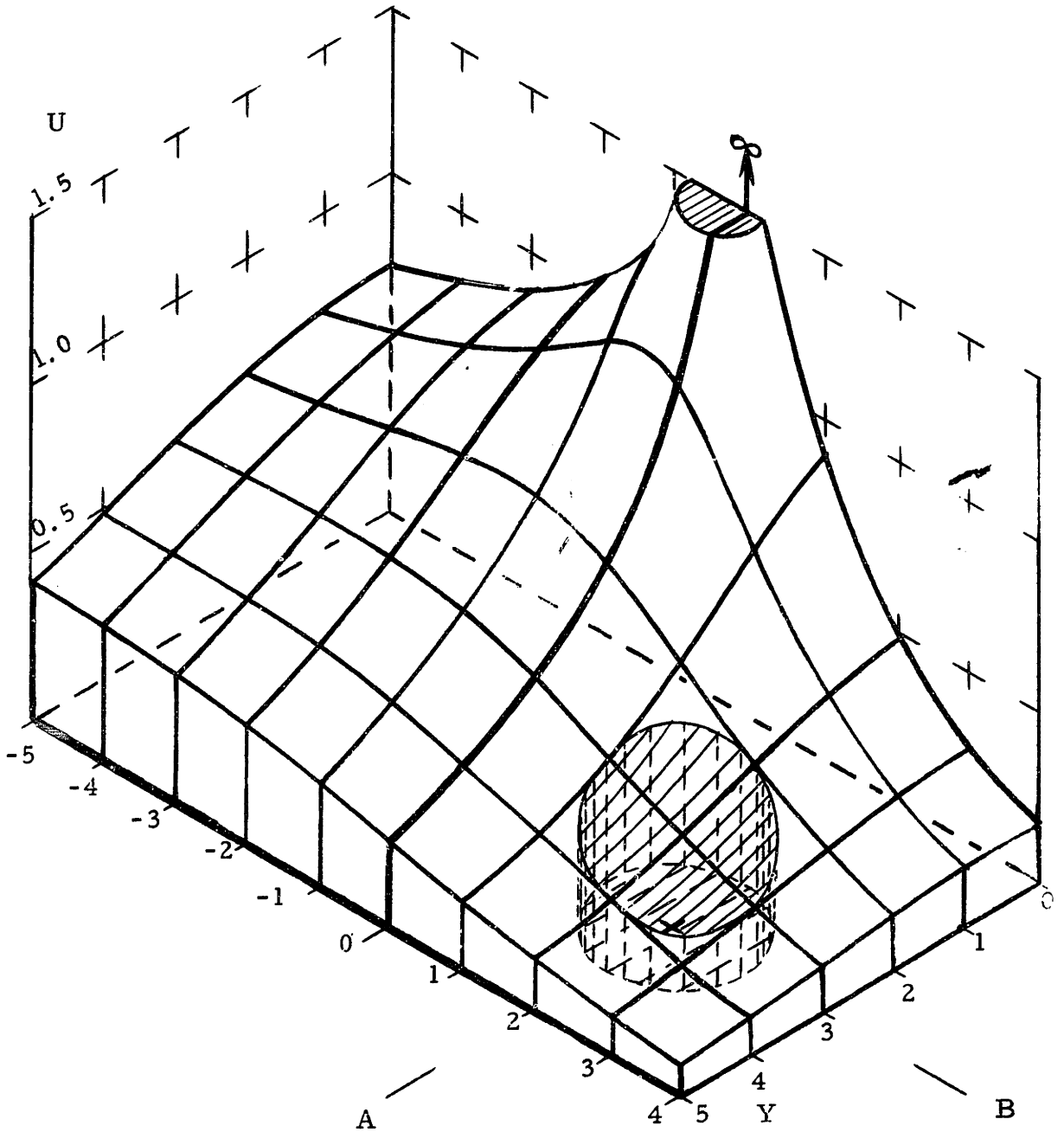


Figure 1: Temperature Surface from Moving Point Source

Surface depicting the temperature on a plane due to a point source of heat located at the origin, and moving in the positive Z direction at velocity $V=0.1$. The Z_1 - Y coordinates move with the source. The temperature observed at point (A,B) due to a uniform circular source centered at the origin is proportional to the shaded-in volume.

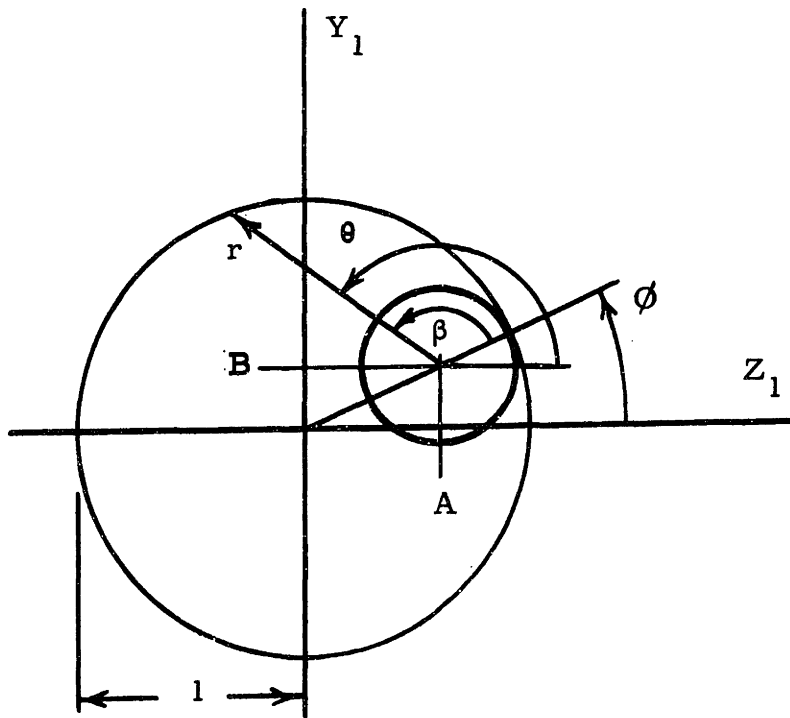


Figure 2

Regions of Integration in Case III

Evaluation of (3-35) in Case III ($\sqrt{A^2 + B^2} < 0.95$). The integral over the smaller circle is given by (3-50). The integral over the area outside the small circle and inside the large circle is given by (5-9).

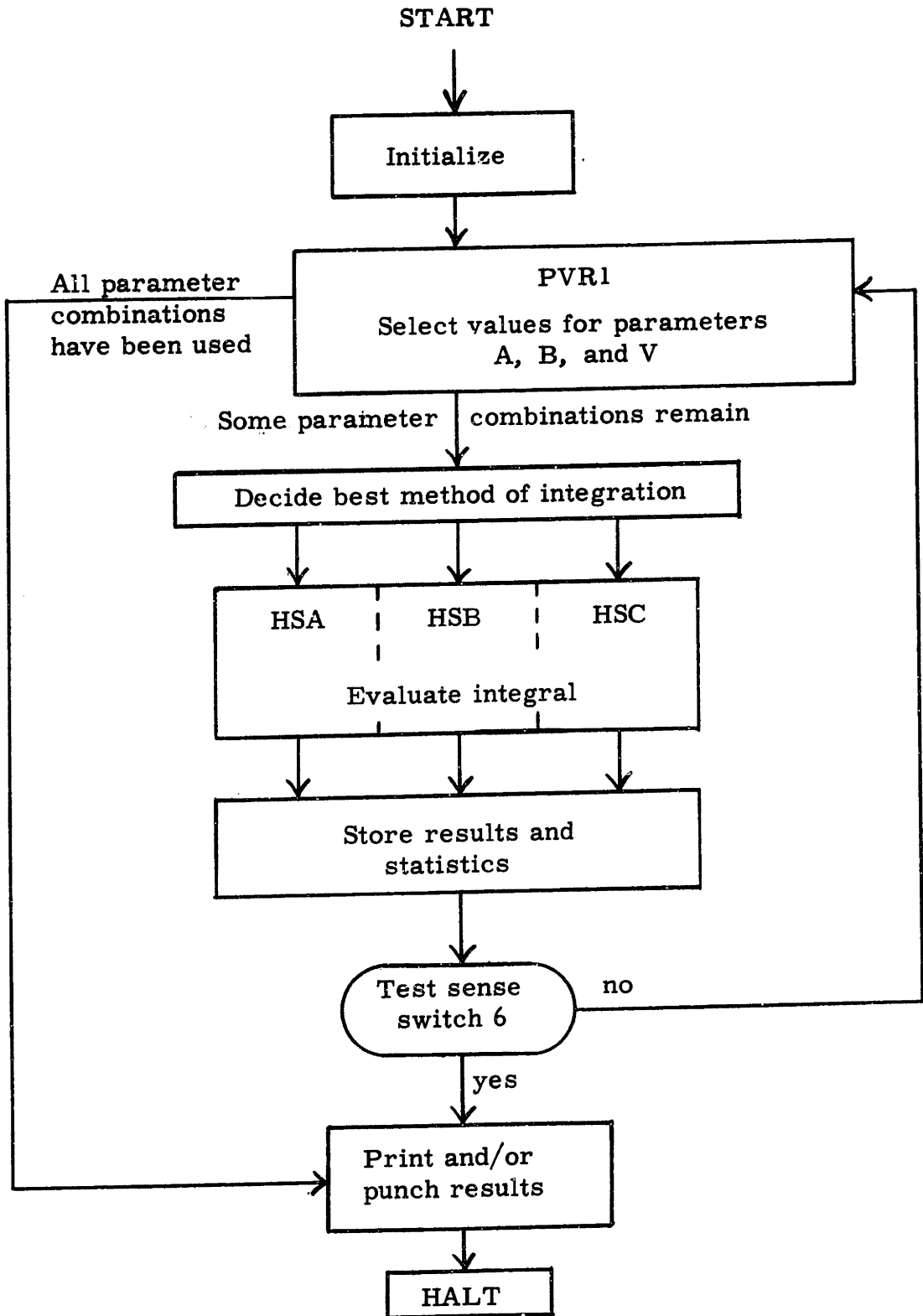


Figure 3

Main Program Flow Diagram

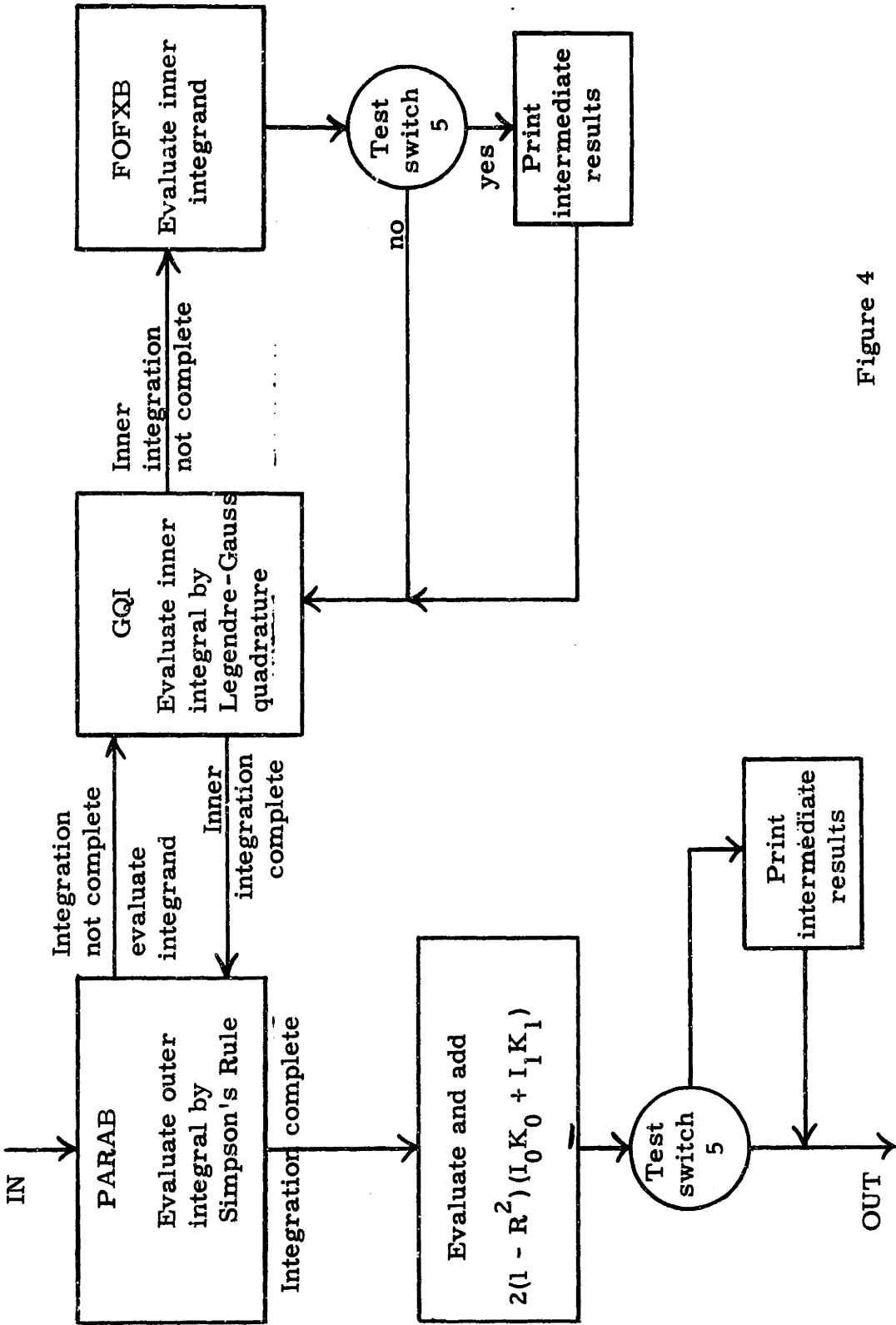


Figure 4

Flow Diagram for Computation of Temperature
in Case III
(Corresponds to subroutine HSB in Figure 3)

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