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ANALYSIS OF A TWO-DIMENSIONAL MASS TRANSPORT PROBLEM IN CONTAMINATION OF SPACE FLIGHT EXPERIMENTS

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16. ABSTRACT

The two-dimensional mass transport problem in a box with sinks and sources is analyzed both analytically and numerically. The results are compared and found to be in good agreement. The basis is thus laid for a three-dimensional numerical (Monte Carlo) mass transport program for use in analysis of space flight contamination experiments.

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INTRODUCTION

The problem of contaminant particles becomes ever more critical as the state of the art advances in space flight experiments involving measurement of optical and ultraviolet radiation. A method of determining contributions from local sources is needed to optimize system performance. Sources such as spacecraft dumps and rocket firings are relatively easy to analyze and isolate from critical surfaces because they are external and discontinuous in time. Outgassing, however, occurs internal to the experiments and continuously in time. Quantities of experimental data on outgassing rates are available, but there has been no effort to apply boundary conditions to make such outgassing data meaningful in a flight situation. The purpose of this study is to make such an application and thereby contribute a vital unit to an optimization program for design of optical flight experiments.

It may be worthwhile here to place this problem in context and point out the interfaces with other subprograms in the optimization program (Fig. 1). The output of the first subprogram will be source rates. This will serve as input to the mass transport subprogram along with sticking coefficients of

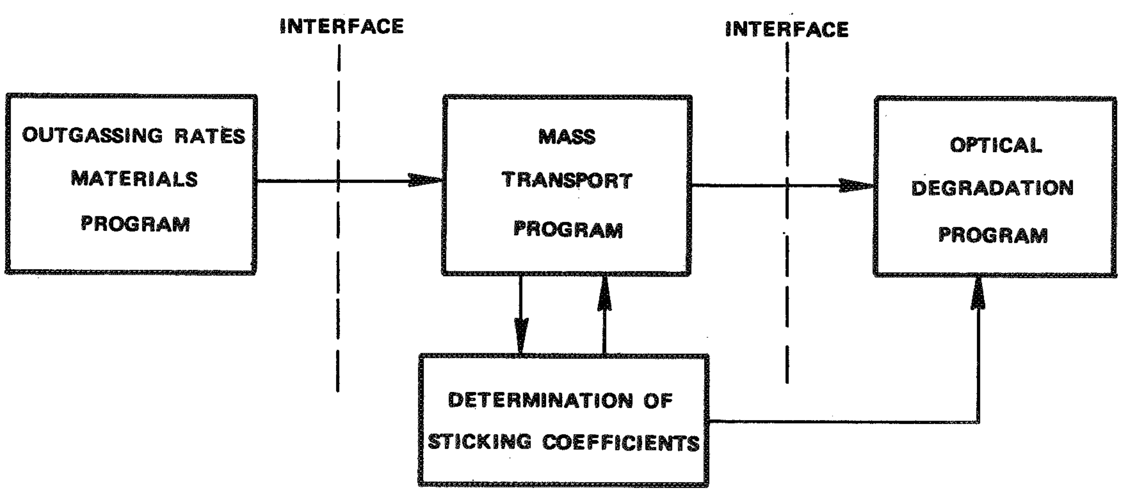


Figure 1. Subprograms in the contamination program.

boundary surfaces. The output of the mass transport analysis will be a mass flux at the optical surface of interest. This will serve as input to an optical degradation program to determine the effects of this flux upon the experiment. All areas shown in Figure 1 are being worked on.

ANALYTIC APPROACH TO THE TWO-DIMENSIONAL CONTAMINATION PROBLEM

The eventual goal of this study was to provide a general design tool for optimizing optical experiments in space. At the time the study was begun the most pressing need for such analysis existed in the Apollo Telescope Mount (ATM) program. For this reason the parameters chosen are meant to exemplify a typical ATM experiment. Even more critical is the altitude for which the calculations are carried out. This altitude determines whether the problem is to be purely geometric or is to involve particle-particle collisions within the experiment itself. At the ATM altitude of 425 kilometers (235 n. mi) the mean free path of a particle is approximately 10^4 meters [1], which essentially dictates a geometric approach. Although pressure in the canister builds up to higher values the lowest value of mean free path with the doors open is approximately 80 meters, which is still a geometric problem. However, the doors are closed during the night cycle, since ATM is a solar experiment, and the pressures build up to values that would result in intermolecular collisions. With the doors closed there is no "wind" and consequently no momentum transfer; therefore, the problem is still basically geometrical in character. The primary effect might be expected to come from the sticking coefficient, but this turns out to be surprisingly pressure independent, [1] and for this reason the increase in pressure during the night does not seem to seriously invalidate the geometric approach. At worst, an effective increase in source rate should handle this problem. There is a compensating factor in that absorption on the lens is less in the absence of ultraviolet radiation.

Calculation of the Probability of Particle Striking Optical Surface After One Collision with Wall

To solve the problem analytically it is necessary to obtain the probability that a re-emitted particle at point x on the wall will strike the lens

1. Conversation with J. F. Scannapieco, General Electric, Valley Forge, Pennsylvania, July 1969.

(Fig. 2). This is simply the ratio of the angle subtended by the lens to the angle into which the particle is emitting. (For three dimensions, it is the ratio of solid angles.) This is with the assumption of isotropic emission. Such an assumption will be replaced by a more realistic distribution as soon as the geometric probability is obtained.

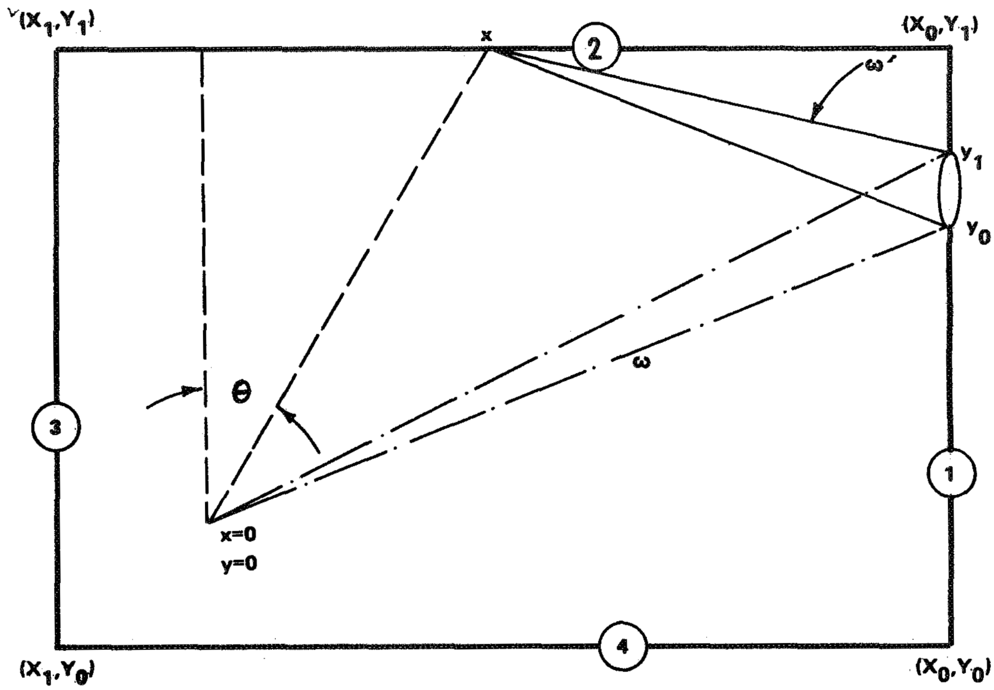


Figure 2. Basic geometry to be considered.

General symbols are defined as follows:

N	the number of particles per second from the source at $(0, 0)$.
N_x	the number of particles per second from the wall at (x, y)
ω	angle subtended by lens referred to the source $(0, 0)$.
ω'	angle subtended by lens referred to point (x, y)

X_0, X_1, Y_0, Y_1	corner points of two-dimensional box
y_0, y_1	boundary of lens
1, 2, 3, 4	the number of the wall for later clarity.

From Figure 2 it is seen that

$$x = Y \quad \tan\theta \quad , \tag{1}$$

and, from the defined quantities, it follows that the number of particles per second which will strike the lens directly from the source is $\frac{\omega}{2\pi}$ N, while from wall 1 there will be $\frac{\omega}{\pi}\ N_x$ particles per second striking the lens. To determine some value for N_x, it is necessary to scale up the part of the drawing concerned with the top wall (Fig. 3).

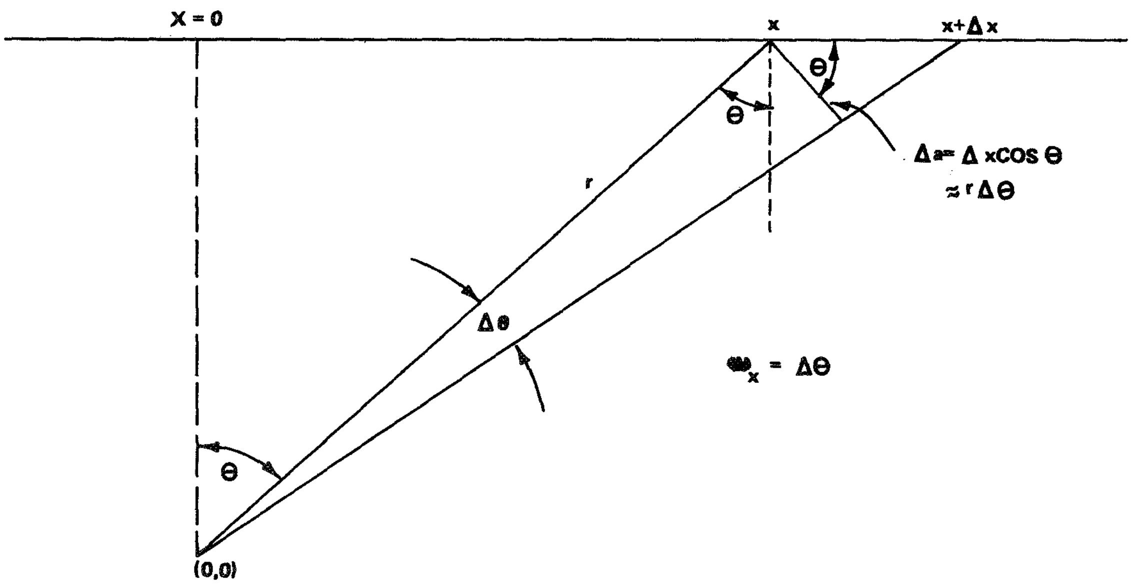


Figure 3. Enlargement of top wall geometry.

From Figure 3 it can be seen that

$$dN_x = N\,\frac{d\theta}{2\pi} \quad ,$$

which gives the number of particles per second hitting at x in the cone $d\theta$.

(Note: 2π radians is to be replaced by 4π steradians in the three-dimensional problem.) The total number of particles that hit between x and x+Δx per second is defined by

$$N_{x,\Delta x} = \int_{x}^{x+\Delta x} dN_x = \frac{N}{2\pi} \int_{\theta(x)}^{\theta(x+\Delta x)} d\theta = \frac{N}{2\pi} \left[\theta(x+\Delta x) - \theta(x)\right] \quad . \qquad (2)$$

From equation (1), it follows that

$$\theta(x) = \tan^{-1}\left(\frac{x}{y}\right)$$

$$\theta(x+\Delta x) = \tan^{-1}\left(\frac{x+\Delta x}{y}\right)$$

A series expansion [2] for the arc tan α is

$$\tan^{-1}\alpha = \alpha - \frac{1}{3}\alpha + \frac{1}{5}\alpha - \frac{1}{7}\alpha + \ldots \quad (\alpha < 1) \qquad (3a)$$

$$= \frac{\pi}{2} - \frac{1}{\alpha} + \frac{1}{3}\frac{1}{\alpha} - \frac{1}{5\alpha} + \ldots \quad (\alpha > 1) \quad . \qquad (3b)$$

Using the formulas to first order in Δx for $x < y$ allows the calculation of

$$\tan^{-1}\left(\frac{x+\Delta x}{y}\right) - \tan^{-1}\left(\frac{x}{y}\right) = \frac{1}{y}\left[\sum_{n=0}\left(\frac{x}{y}\right)^{2n}(-1)^{n}\right]\Delta x \text{ for } x < y \quad . \ (4)$$

Consider the case $x > y$

$$\tan^{-1}\left(\frac{x+\Delta x}{y}\right) = \frac{\pi}{2} - \frac{y}{x}\left(1 + \frac{\Delta x}{x}\right)^{-1} + \frac{1}{3}\left(\frac{y}{x}\right)^{3} \times \left(1 + \frac{\Delta x}{x}\right)^{-3} - \frac{1}{5}\left(\frac{y}{x}\right)^{5}\left(1 + \frac{\Delta x}{x}\right)^{-5} + \ldots$$

Here it is necessary to use the binomial theorem,

$$\lim_{\Delta x \to 0} (1+\Delta x)^n \simeq 1 + n\Delta x \quad ,$$

to obtain

$$\tan^{-1}\left(\frac{x+\Delta x}{y}\right) = \frac{\Pi}{2} - \frac{y}{x}\left(1 - \frac{\Delta x}{x}\right) + \frac{1}{3}\left(\frac{y}{x}\right)^3\left(1 - \frac{3\Delta x}{x}\right)$$
$$- \frac{1}{5}\left(\frac{y}{x}\right)^5\left(1 - \frac{5\Delta x}{x}\right) + \ldots$$

Therefore, to first order in Δx, equation (5) is obtained:

$$\tan^{-1}\left(\frac{x+\Delta x}{y}\right) - \tan^{-1}\left(\frac{x}{y}\right) = \frac{1}{y}\left[\sum_{n=1}^{\infty} (-1)^{n+1}\left(\frac{y}{x}\right)^{2n}\right]\Delta x \text{ for } x > y \quad . \tag{5}$$

It is possible to put these expressions in a closed form by observing that

$$\lim_{\Delta x \to 0} \frac{\tan^{-1}(x+\Delta x) - \tan^{-1}(x)}{\Delta x} = \frac{d}{dx}\tan^{-1}(x)$$

and

$$\frac{d}{dx}\tan^{-1} u = \frac{1}{1+u^2}\frac{du}{dx} \quad \text{or} \quad d\left[\tan^{-1}\left(\frac{x}{y}\right)\right] = \frac{1}{y}\left(\frac{1}{1+\frac{x^2}{y^2}}\right)dx \quad .$$

By rewriting equation (4) in a simple form through the use of complex notation and comparing this to the geometric series, it can be noted that, for $x < y$,

$$\left[\tan^{-1}\left(\frac{x+\Delta x}{y}\right) - \tan^{-1}\left(\frac{x}{y}\right)\right] = \frac{\Delta x}{y}\left\{\sum_{n=0}^{\infty}\left[\left(\frac{ix}{y}\right)^2\right]^n\right\} = \frac{\Delta x}{y}\,\frac{1}{1-\left(\frac{ix}{y}\right)^2}$$
$$= \frac{y\Delta x}{x^2+y^2} = \Delta\tan^{-1}\left(\frac{x}{y}\right) ,$$

and for $x > y$

$$\left[\tan^{-1}\left(\frac{x+\Delta x}{y}\right) - \tan^{-1}\left(\frac{x}{y}\right)\right] = \frac{-\Delta x}{y}\left\{\sum_{n=1}^{\infty}\left[\left(\frac{iy}{x}\right)^2\right]^n\right\} = \frac{-\Delta x}{y}\left\{\sum_{n=0}^{\infty}\left[\left(\frac{iy}{x}\right)^2\right]^n - 1\right\}$$

$$= \frac{-\Delta x}{y}\left[\frac{1}{\left(1 + \frac{y^2}{x^2}\right)} - 1\right]$$

$$= \frac{y\Delta x}{x^2 + y^2} = \Delta\tan^{-1}\left(\frac{x}{y}\right) .$$

From equation (2), it follows that

$$N_{x,\Delta x} = \frac{N}{2\pi}\,\frac{y\Delta x}{x^2 + y^2} \tag{6}$$

for all values of $\left(\frac{x}{y}\right)$. As mentioned earlier, this number is for assumed isotropic re-emission off the wall. This is not a very good assumption and will now be replaced by a directionally dependent probability factor. A cosine dependence which is illustrated schematically in Figure 4 will be used.

To make an application of this directional dependence to the top wall shown in Figure 2, it is necessary to analyze the geometry in more detail (Fig. 5). The definition of several parameters shown in Figure 5 are

$$y' = \frac{y_1 + y_0}{2} \quad ;$$

$$\theta = \tan^{-1}\left(\frac{Y_1 - y}{X_0 - x}\right) \quad ;$$

$$S = |y_1 - y_0| \cos\theta \quad ;$$

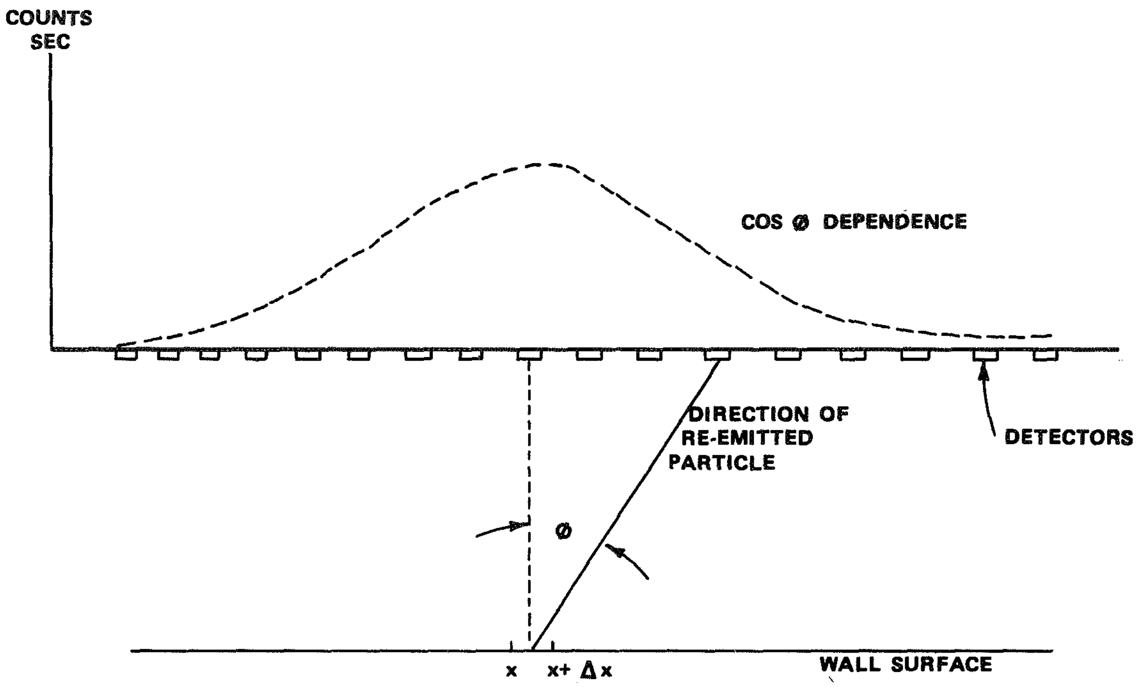


Figure 4. Illustration of meaning of cosΦ dependence.

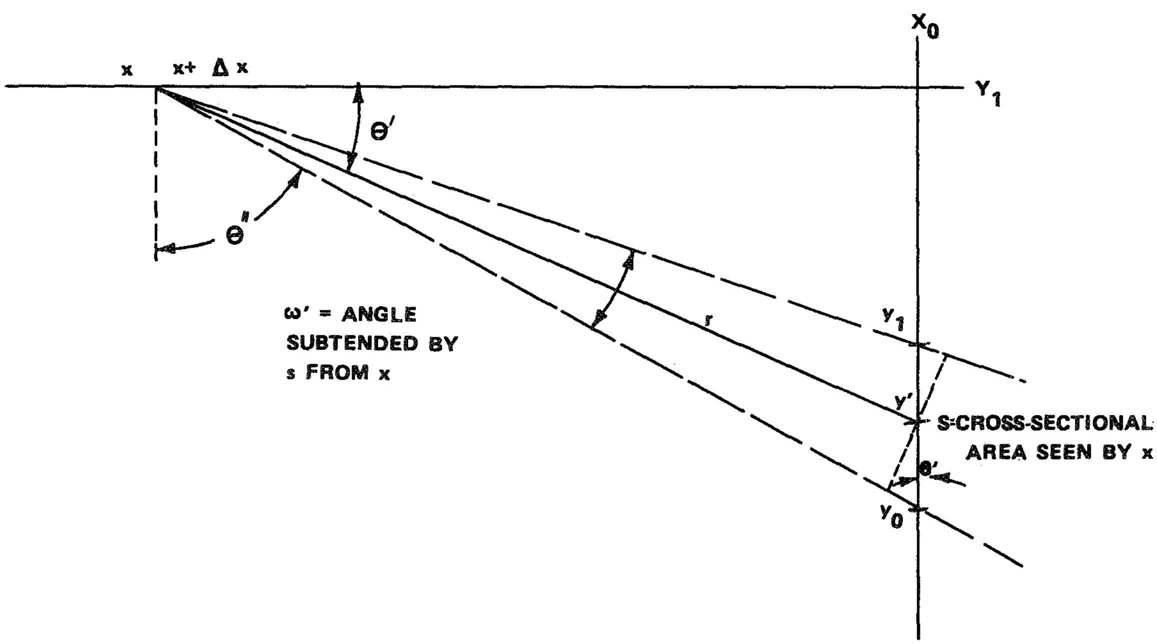


Figure 5. Geometry from which the directional dependence is derived.

$$\omega' = \frac{s}{r} = \frac{|y_1 - y_0| \cos \tan^{-1}\left(\frac{Y_1 - y}{X_0 - x}\right)}{\sqrt{(X_0 - x)^2 + (Y_1 - y')^2}} \quad ;$$

$$\theta'' = \frac{\pi}{2} - \theta' \quad . \tag{7}$$

If it is assumed that all particles are re-emitted from Δx, the number of particles per second leaving in the direction θ'' is proportional to $\cos\theta''$. Denote the number per second leaving Δx in direction θ by $N_{\Delta x, \theta} = N_{\Delta x}$ $\cos\theta$. The sum over all directions must be the total number leaving $N_{x, \Delta x}$; i.e.,

$$\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} N_{\Delta x, \theta} d\theta = N_{x, \Delta x} = N_{\Delta x} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \cos\theta \, d\theta = 2 N_{\Delta x} \quad . \tag{8}$$

Therefore,

$$N_{\Delta x} = \frac{N_{x, \Delta x}}{2} \quad \text{and} \quad N_{\Delta x, \theta} = \frac{1}{2} N_{x, \Delta x} \cos\theta$$

is the normalized distribution that gives the angular dependence of particles leaving Δx.

It is necessary to modify the preceding results slightly to take into account the fact that some particles permanently stick to the walls and are not re-emitted. For this purpose a new parameter P will be defined to be the probability that a particle will be re-emitted from the surface. This P may be a function of temperature or other variables, but it is not necessary to specify such dependence at this point. The particles leaving the surface are then reduced by a factor P. It should be noticed that 1-P would correspond to the percentage (or probability) of particles sticking permanently to the surface and will be called the sticking coefficient. Under equilibrium conditions it is then possible to specify the number of particles emitted from Δx(at x) into the angle ω(at θ). This is the number of particles leaving Δx(at x) that will hit the optical surface,

$$N_{\Delta x\ \text{lens}} = N_{\Delta x,\theta''}\frac{\omega}{\pi} = \frac{P}{2} N_{x,\Delta x} \cos\theta'' \frac{(s/r)}{\pi} .$$

In two dimensions the number of particles leaving the source, going to x, being re-emitted randomly with d'Lambertian distribution and hitting the lens is

$$N_{\text{source} \xrightarrow{\Delta x} \text{lens}} = \frac{P}{2} N_{x,\Delta x} \cos\theta \frac{|y_1-y_0| \cos\theta'}{\pi\left[(X_0-x)^2 + (Y_1-y')^2\right]^{1/2}} . \tag{9}$$

Although the cosine dependence is explicit in $\cos\theta''$, it is preferable to employ the relationship $\cos\left(\frac{\pi}{2} - \theta'\right) = \sin\theta'$ and use the expression for θ' given in equation (7). The expression for $N_{x,\Delta x}$ for the particles hitting in the region Δx has already been given [equation (6)] in terms of the source rate and geometry. Substituting these expressions into equation (9) yields

$$N_{\text{source} \xrightarrow{\Delta x} \text{lens}} = \frac{PN}{(2\pi)^2} \frac{|y_1-y_0|\ Y_1 \sin\tan^{-1}\left(\frac{Y_1-y'}{X_0-x}\right) \cos\tan^{-1}\left(\frac{Y_1-y'}{X_0-x}\right)}{(x^2+Y_1^2)\sqrt{(X_0-x)^2+(Y_1-y')^2}} . \tag{10}$$

To consider all the particles from the source which make only <u>one</u> collision with the "top" (or "bottom") wall and proceed to the lens it is necessary to integrate over the top (or bottom with appropriate geometry) wall:

$$N_{\text{top} \xrightarrow{1} \text{lens}} = \frac{PN|y_1-y_0|Y_1}{(2\pi)^2} \int_{X_1}^{X_0} \frac{\sin\tan^{-1}\left(\frac{Y_1-y'}{X_0-x}\right) \cos\tan^{-1}\left(\frac{Y_1-y'}{X_0-x}\right) dx}{(x^2+Y_1^2)\sqrt{(X_0-x)^2 + (Y_1-y')^2}} . \tag{11}$$

Before treating the case in which the particle makes more than one collision with the walls and then hits the lens it is necessary to consider the "back" wall (wall 3). The geometry for this case is shown in Figure 6.

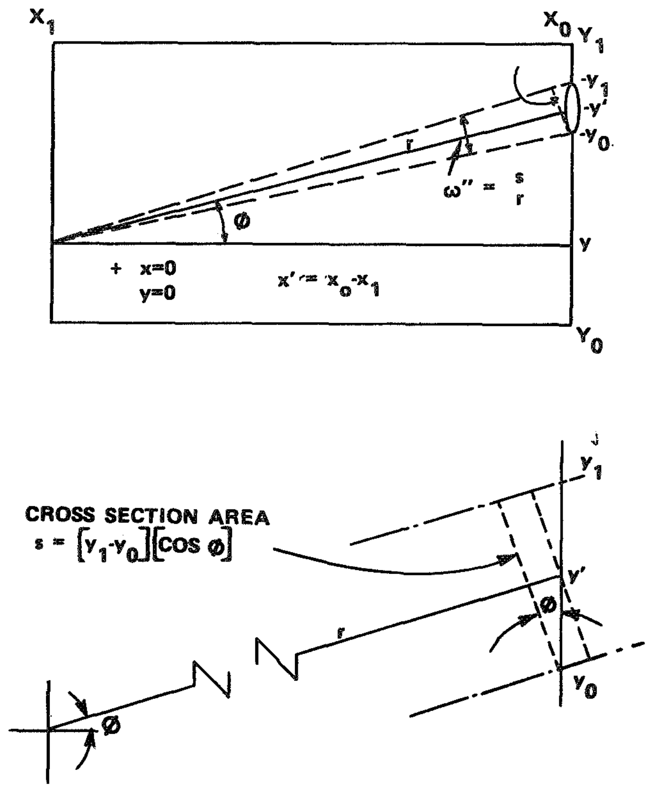


Figure 6. Geometry of back wall contributions.

The distance from the Δy region on the back wall to the center of the lens is given by

$$r = \sqrt{x'^2 + (y' - y)^2} = \sqrt{x'^2 + y''^2} \quad ,$$

and the angle Φ is given by

$$\Phi = \tan^{-1}\left(\frac{y''}{x'}\right) \quad .$$

As previously determined the number of particles per second leaving the Δy "area" is $PN_{y,\Delta y}$, where $N_{y,\Delta y}$ has been defined for the back wall analogously to $N_{x,\Delta x}$ for the top wall. The number leaving in the direction Φ is proportional to $\cos\Phi$. After normalizing, as in equation (8), this number is seen to be

$$N_{\Delta y,\Phi} = \frac{P}{2} N_{y,\Delta y} \cos\Phi \quad .$$

For random Φ the probability of a particle hitting the lens is

$$N_{\Delta y \to \text{lens}} = N_{\Delta y,\Phi}\left(\frac{\omega''}{\pi}\right) = N_{\Delta y,\Phi} \frac{|y_1 - y_0| \cos \tan^{-1}\left(\frac{y''}{x'}\right)}{\pi\sqrt{x'^2 + y''^2}}$$

When the last two equations are combined, the number of particles leaving the source, hitting Δy, and re-emitting to strike the lens is seen to be

$$N_{\text{source} \xrightarrow{\Delta y} \text{lens}} = \frac{P}{2\pi} N_{y,\Delta y} \frac{|y_1 - y_0| \cos^2 \tan^{-1}\left(\frac{y''}{x'}\right)}{\sqrt{x'^2 + y''^2}} \quad . \tag{12}$$

The number of particles leaving the source and striking Δy is found in the same manner that the number striking Δx was determined. Thus,

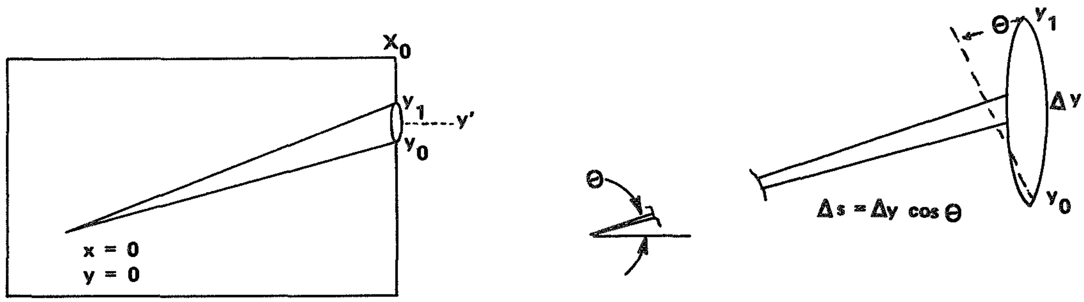
$$N_{y,\Delta y} = \frac{N}{2\pi} \frac{x'\Delta y}{x'^2 + y''^2} \quad .$$

This is substituted into equation (12). To find the total contribution from the back wall of particles making only <u>one</u> collision and proceeding to the lens, the sum over all Δy's is taken. In the limit this sum becomes the integral

$$N_{\text{back} \xrightarrow{1} \text{lens}} = \frac{PN|X_0 - X_1||y_1 - y_0|}{(2\pi)^2} \int_{Y_0}^{Y_1} \frac{\cos^2 \tan^{-1}\left(\frac{y'-y}{X_0 - X_1}\right) dy}{[(X_0 - X_1)^2 - (y'-y)^2]^{3/2}} \quad . \tag{13}$$

The one-collision contributions from the top and back walls have been determined. The bottom wall is simply treated as a top wall and equation (11) is used with appropriate geometry. Since only straightline paths are assumed there can be no single-collision contribution from the front wall. The contribution from the source directly to the lens will now be calculated. The geometry is shown in Figure 7.

The direct contribution to the lens is proportional to the angle subtended by the lens divided by the angle into which the source is isentropically emitting, that is, $\omega/2\pi$, where



(a) (b)

Figure 7. Source to lens geometry.

$$\omega = \int \frac{\Delta s}{r} = \int_{Y_0}^{Y_1} \frac{\Delta y \cos\theta}{r} = \int_{Y_0}^{Y_1} \frac{X_0 \Delta y}{X_0^2+y^2} = \tan^{-1}\left(\frac{y_1}{X_0}\right) - \tan^{-1}\left(\frac{y_0}{X_0}\right)$$

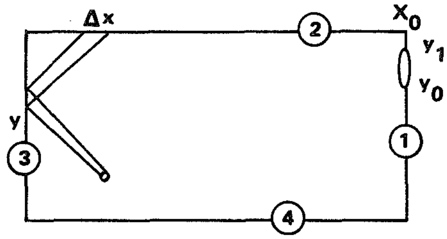
For a source emitting N particles per second into 2π radians for $\Delta y << x_0$ this expression is reducible to [See equation (6)]:

$$N_{\text{source} \rightarrow \text{lens}} \simeq \frac{N}{2\pi} \frac{|y_1 - y_0| X_0}{X^2 + y'^2} \quad \text{for } \Delta y << x_0 \ . \tag{14}$$

At this point, calculations are possible and have been carried out for typical geometries. These will be compared to a more realistic solution which is considered in the next subsection.

Calculation of the Probability of a Particle Striking the Optical Element After Two Collisions with Intermediate Surfaces

The contribution to the optical surface from particles striking a surface element and being re-emitted has been found. All particles on this surface element were assumed to have come directly from the source; but actually some of the particles on any surface element have reached their position after at least one collision with another wall. The special case in which only one prior collision is assumed will be treated by the following procedure: Let the surface element in question be area Δx on the top wall. By treating this element as an optical surface the technique developed in the previous subsection can be used to find the contributions to this element from particles making one collision with another wall prior to striking the surface. It is necessary to make the identification of Δx with $|y_1 - y_0|$ in equations (11) and (13) and to modify other parameters to fit the format of these equations. Symmetry arguments allow all possible wall combinations to be handled with only two basic calculational techniques. Both basic configurations are represented in Figure 8.



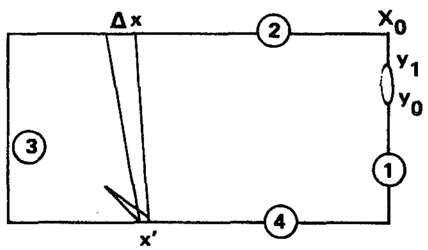


Figure 8. Geometry involved in determining number of particles making one collision with the walls before striking x.

The geometries shown in Figure 8 must be rotated through 90 degrees to be put in a format which is obviously suited for application of equations (11) and (13). The rotated geometrics are shown and labeled in Figure 9.

It should be obvious from inspection of the above figures that the words "top" and "bottom" and "front" and "back" are interchangeable. All possible combinations of two wall collisions are handled by equations (11) and (13) with conversion of the figures to the appropriate formats.

For purposes of calculation it is necessary to choose some sample geometry. The geometry shown in Figure 10 will be that used for all calculations in this report.

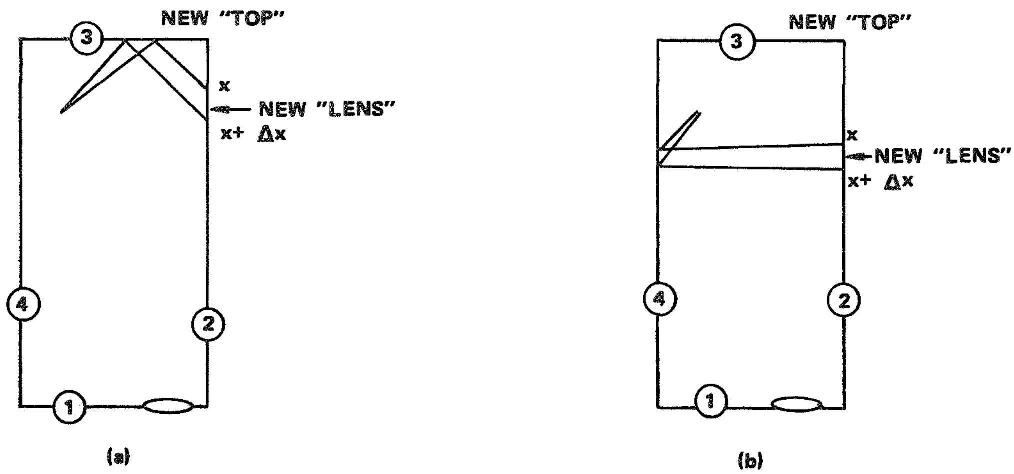


Figure 9. Conversion of Figure 8 to required formats.

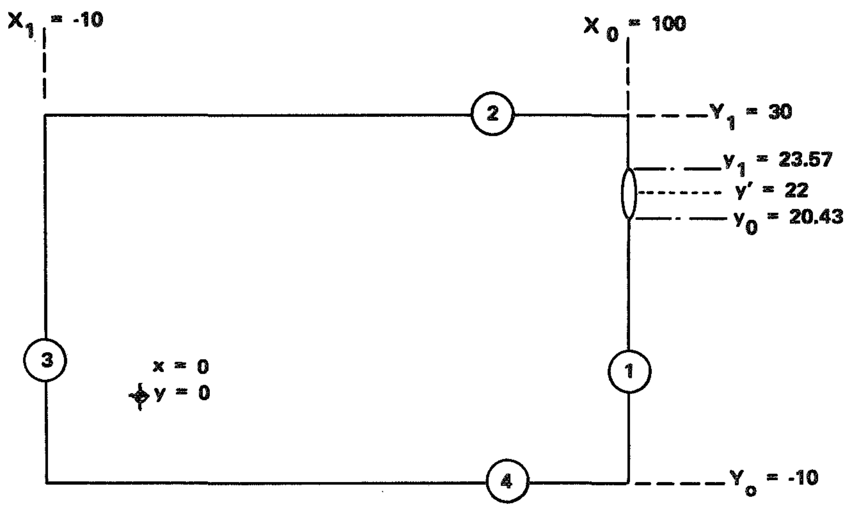


Figure 10. Values used in all calculations (all distances in centimeters).

Calculations have been performed for the configuration shown in Figure 9a with the distances given in Figure 10. It is reasonable to assume that the one-collision contributions to Δx depend on the location of Δx and this is found to be true. Therefore, Δx was located at seven different points ranging completely over the top wall. The contributions from wall 3 to Δx on wall 2 were found to vary smoothly with x and assumed values from 0.000132 $PN\Delta x$ to 0.000663 $PN\Delta x$. A curve was fitted to the points such that the contribution found by equation (11) can be represented as

$$N_{3\rightarrow\Delta x \text{ on } 2} = k_1(x)\ PN\Delta x \quad , \tag{15}$$

where

$k_1(x) = 0.000703 - 0.0000107x + 0.000000044x^2$

P = probability that particle will re-emit from wall 3

N = number of particles per second emitted by source

Δx = area of surface element on wall 2

$N_{3\rightarrow\Delta x \text{ on } 2}$ = particles emitted from wall 3 to Δx on wall 2.

A very good approximation to equation (15) is

$$N_{\text{wall } 3\rightarrow\Delta x \text{ on } 2} \simeq 0.0004\ PN\Delta x \tag{16}$$

Similar calculations for the contribution to Δx on wall 2 from those particles which leave the source, strike wall 4, are re-emitted, and proceed on the Δx have been carried out as above. The configuration is that corresponding to Figures 8b and 9b and the relevant formula is equation (13) with appropriate parameters. The results of moving Δx along wall 2 are given on the basis of nine points. These nine points yielded contributions to Δx varying smoothly from 0.000419 $PN\Delta x$ to 0.000798 $PN\Delta x$. A curve fit program yielded

$$N_{4\rightarrow\Delta x \text{ on } 2} = k_1(x)\ PN\Delta x \quad ,$$

where the symbols are explained above and the dependence on the location of Δx on wall 2 is best described by

$k_1(x) = 0.0005605 + 0.0000113x - 0.0000001x^2$

A very good approximation to $N_{4\rightarrow\Delta x \text{ on } 2}$ is given by

$$N_{4\rightarrow\Delta x \text{ on } 2} \approx 0.0007\ PN\Delta x \quad . \tag{17}$$

In a similar manner, symmetry considerations allow the calculation of the contribution to Δx from the front wall. The results found on the basis of seven points can be summarized by

$$N_{1\to\Delta x \text{ on } 2} \approx 0.00009\, PN\Delta x \tag{18}$$

By extending consideration to those particles which make 2, 3, 4, or more collisions with various walls before landing in the region from x to $x+\Delta x$ on wall 2, it is possible to write an expression for the number of particles striking Δx per second:

$$N_{x,\Delta x} \underbrace{\int_x^{x+\Delta x} dN_x}_{\text{direct}} + P \underbrace{\int_x^{x+\Delta x} dN_{1x}}_{\text{one collision}} + P^2 \underbrace{\int_x^{x+\Delta x} dN_{2x}}_{\text{two collisions}}$$

$$+ P^3 \underbrace{\int_x^{x+\Delta x} dN_{3x}}_{\text{three collisions}} + \ldots + P^n \underbrace{\int_x^{x+\Delta x} dN_{nx}}_{\text{n collisions}} + \ldots$$

The first integral represents the direct contribution to Δx from the source and has already been integrated [equation (14)], and the second integral represents the one collision contribution expressed in equations (16), (17), and (18). A similar notation is adopted for the remainder of the series after integration such that

$$N_{x,\Delta x} = N\left[\frac{y}{2\pi\,(x^2+y^2)}\,\Delta x + P k_1(x)\Delta x + P^2 k_2(x)\Delta x + \ldots\right.$$

$$\left. + P^n k_n(x)\Delta x + \ldots\right] \tag{19}$$

The maximum value of $P=1$ for which the series diverges represents the physically unrealizable situation in which no particles ever stick to the surfaces. All other values of P lead to convergent series, assuming that $k_n(x)$ are well-behaved. It will also be assumed that the following relation holds:

$$k_{n+1}(x) \le k_n(x) \tag{20}$$

Before an attempt is made to sum this series, the situation in which there are holes in the container walls will be considered. Although each hole must be separately considered as a possible source of contaminant particles, it also serves as a sink for particles. If the area of the sinks is denoted by a and the area of the container walls denoted by A, the probability of an arbitrary particle re-emitting and striking Δx is decreased by $\frac{A}{A+a}$. This is only approximately exact but the error does not justify the effort necessary to find the exact effect which would be a function of the walls on which the particles, Δx, and the sinks were located. If this factor is taken into account in the definition

$$P' = P\left(\frac{A}{a+A}\right)$$

and if this probability is used in equation (19), the equation becomes

$$N_{x,\Delta x} = N_{\Delta x}\left[\frac{y}{2\pi(x^2+y^2)} + \sum_{n+1}^{\infty} k_n(x)\, P'^n\right] \tag{21}$$

The relation given by equation (20) establishes an upper bound to the series. If the equality is chosen, the series becomes a geometric series in P' after factoring out $k_1(x)\, P'$ from equation (21). This maximum contribution to Δx at x is given by

$$N_{x,\Delta x} = N\Delta x\left[\frac{y}{2\pi(x^2+y^2)} + \frac{k_1(x)\, P'^2}{1-P'}\right] \tag{22}$$

This value can now be substituted into equation (9) to give the contribution to the lens from the top (bottom) wall taking all collisions into consideration. Thus, equation (11) can be rewritten as follows:

$$N_{top\rightarrow lens} = \frac{PN|y_1-y_0|}{(2\pi)^2}\int_{X_1}^{X_0}\left[\frac{Y_1}{x^2+y_1^2} + \frac{2\pi\, k_1(x)\, P'^2}{1-P'}\right] \times \frac{\sin\tan^{-1}\frac{Y_1-y'}{X_0-x}\ \cos\tan^{-1}\frac{Y_1-y'}{X_0-x}\ dx}{\sqrt{(X_0-x)^2+(Y_1-y')^2}} . \tag{23}$$

In a similar manner equation (21) can be substituted into equation (12) for the contribution to the lens from the back wall. All collisions are considered. This allows equation (13) to be rewritten:

$$N_{\text{back}\rightarrow\text{lens}} = \frac{PN|y_1-y_0|}{(2\pi)^2} \int_{Y_0}^{Y_1} \left[\frac{X_0 - X_1}{(X_0-X_1)^2 + (y'-y)^2} + \frac{2\pi\, k_1(x)\, P'^2}{1 - P'}\right] \frac{\cos^2 \tan^{-1}\left(\frac{y'-y}{X_0-X_1}\right) dy}{\sqrt{(X_0-X_1)^2 + (y'-y)^2}} \tag{24}$$

A Simpson's rule numerical integration has been carried out for equations (23) and (24). Some value of $k_1(x)$ must be decided upon before the integral is evaluated. The values in equations (16), (17), and (18) add up to a value of 0.0013 for k_1. All walls are considered. Because this value is low, the integration will be carried out by using several times this number; i.e.,

$$k_1 \simeq 0.0065 \quad .$$

Although the determination of k_1 is the weakest link in the analysis, further work has shown that the above choice of k_1 agrees very well with data obtained by an entirely different approach.

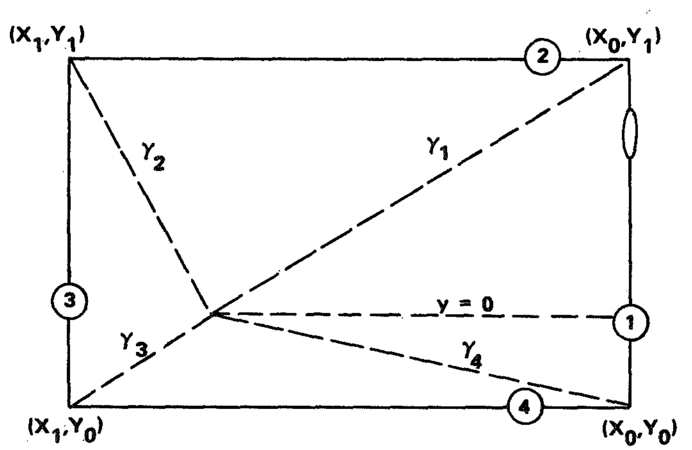
The different approach to the problem is to try a Monte Carlo simulation to be run on a digital computer and compare the results of the analytic and simulation methods. The comparison of results will follow the next section on the Monte Carlo approach.

MONTE CARLO MASS TRANSPORT PROGRAM FOR CONTAMINANT PARTICLES ORIGINATING AT A POINT SOURCE

Because of the extreme difficulty encountered in rigorously determining a value of $k_n(x)$, the extended source function for particles making n collisions before striking Δx, it was decided to check the approximation made with a different approach to the problem. Although the choice of $k_n(x)$ turned out to be very good indeed, the Monte Carlo program was found to have a number of advantages over the analytic one, as might have been imagined. These will be discussed after presentation of the program.

The approach followed is that of generating particles with the required probability distributions and following their motions, keeping track of position at every collision with the walls. At each collision a probability that the individual particle will stick is generated and this is compared with the sticking coefficient. If the particle sticks, a new particle is generated; if not, then the particle leaves the wall with the required directional distribution and the process is repeated. Generating large numbers of particles builds up statistics which provide the desired data.

Since velocities are of no significance for this part of the problem, only directions are generated for each particle. Starting at the source, the space inside the container is divided into quadrants (Fig. 11).



$$\gamma_1 = \tan^{-1}\left(\frac{Y_1}{X_0}\right)$$

$$\gamma_2 = \tan^{-1}\left(\frac{Y_1}{X_1}\right)$$

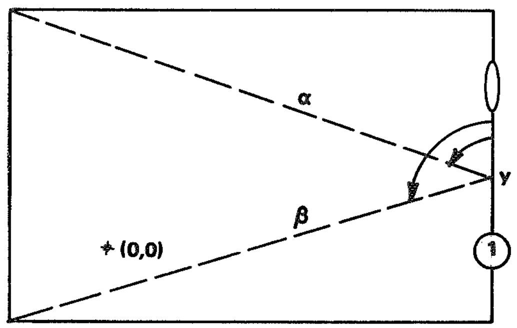
$$\gamma_3 = \tan^{-1}\left(\frac{Y_0}{X_1}\right)$$

$$\gamma_4 = \tan^{-1}\left(\frac{Y_0}{X_0}\right)$$

Figure 11. Quadrants to determine first wall hit.

For each particle a direction is generated and then tested to determine into which quadrant the particle was emitted. Once this determination has been made it is simple trigonometry to calculate the position where the particle strikes the wall. If the particle is to be re-emitted then a new determination of quadrants is necessary if it is to be known which wall the particle will strike. Such a calculation is necessary for every collision since the angles change as a function of position on the wall. Every time the first wall is hit, a check is made to find out if the particle hits the lens. Every time a particle hits the lens, this fact is recorded and a new particle is generated at the source.

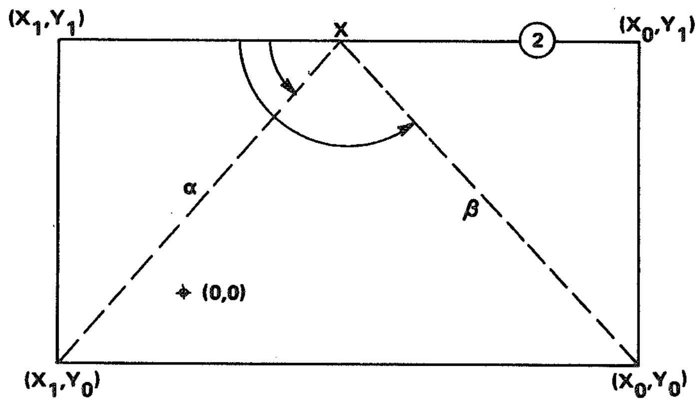
The equation and figures for a particle impinging on each wall are given in Figures 12 through 15. They start with wall 1 and proceed to the next higher number.



$$\alpha = \tan^{-1}\left(\frac{X_0 - X_1}{Y_1 - y}\right)$$

$$\beta = \tan^{-1}\left(\frac{X_0 - X_1}{Y_0 - y}\right)$$

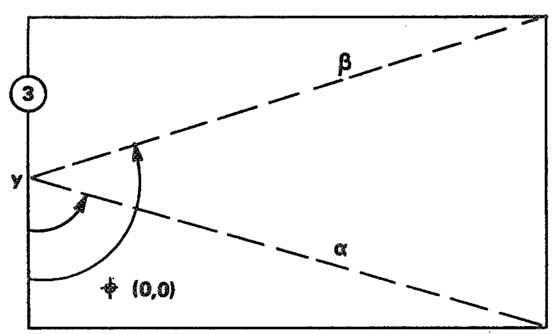
Figure 12. Quadrants for first wall re-emission.



$$\alpha = \tan^{-1}\left(\frac{Y_0 - Y_1}{X_1 - x}\right)$$

$$\beta = \tan^{-1}\left(\frac{Y_0 - Y_1}{X_0 - x}\right)$$

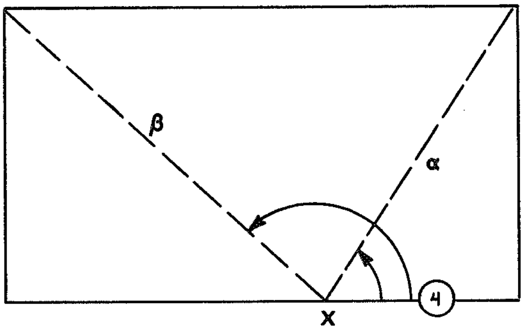
Figure 13. Quadrants for second wall re-emission.



$$\alpha = \tan^{-1}\left(\frac{X_0 - X_1}{y - Y_0}\right)$$

$$\beta = \tan^{-1}\left(\frac{X_0 - X_1}{y - Y_1}\right)$$

Figure 14. Quadrants for third wall re-emission.



$$\alpha = \tan^{-1}\left(\frac{Y_1 - Y_0}{X_0 - X}\right)$$

$$\beta = \tan^{-1}\left(\frac{Y_1 - Y_0}{X_1 - X}\right)$$

Figure 15. Quadrants for fourth wall re-emission.

Every particle which is re-emitted is given a cosine distribution which maximizes the probability of coming off perpendicular to the walls. However, the chance that it may go either to the right or to the left requires a test to see which wall it will hit. This is done by testing on the appropriate α and β given in the above figures. For each wall, then, a new calculation is necessary to ascertain where the particle hit. This is done by trigonometry and results in the following sets of equations:

For a particle coming off wall 1 at position y with angle θ

if $\theta<\alpha$	$x = X_0 + (y-Y_0)\tan\theta$	on wall 2
if $\alpha<\theta<\beta$	$y = y+(X_0-X_1)/\tan\theta$	on wall 3
if $\theta>\beta$	$x = X_0 +(y-Y_1)\tan\theta$	on wall 4 .

For a particle coming off of wall 2 at position x with angle θ

if $\theta<\alpha$	$y = Y_1 +(X_1-x)\tan\theta$	on wall 3
if $\alpha<\theta<\beta$	$x = x+(Y_0-Y_1)/\tan\theta$	on wall 4
if $\theta>\beta$	$y = Y_1+(X_0-x) \tan\theta$	on wall 1 .

For a particle leaving position y on wall 3 with angle θ

if $\theta<\alpha$	$x = X_0 +(y-Y_0)\tan\theta$	on wall 4
if $\alpha<\theta<\beta$	$y = y +(X_1-X_0)/\tan\theta$	on wall 1
if $\theta>\beta$	$x = X_1 +(y-Y_1)\tan\theta$	on wall 2 .

For a particle leaving position x on wall 4 with angle θ

if $\theta<\alpha$	$y = Y_0 + (X_0 - x)\tan\theta$	on wall 1
if $\alpha<\theta<\beta$	$x = x + (Y_1 - Y_0)/\tan\theta$	on wall 2
if $\theta>\beta$	$y = Y_0 + (X_1 - x)\tan\theta$	on wall 3 .

The primary task of the computer is simply to keep track of where the particle is as it generates new random directions for the particle. The data are generated by counting particles emitted versus particles which hit the lens. Although this is the only output of the analytic program, it is also possible to find the mean number of collisions for a given sticking coefficient and to separate the contributions by wall.

The advantages of the Monte Carlo technique over the analytic method are twofold. It is just as easy to consider a source on one of the walls as an interior source with the Monte Carlo. Because the source is always at the origin of the coordinate system, the program decides from the geometry where the source is and handles the situation accordingly. A further advantage is that the thermal distribution is more easily handled in the Monte Carlo case. The sticking coefficient is temperature dependent and this ability may be necessary if there are appreciable thermal changes in the walls as a function of position.

If in the future it is necessary to incorporate baffles into the design, this would be almost impossible with the analytic approach. Although it would not be an easy task, it could probably be written into the Monte Carlo program.

COMPARISON OF RESULTS OF THE MONTE CARLO AND ANALYTIC CALCULATIONS AND CONCLUSIONS

Figures 16 through 19 illustrate the agreement between the two different methods of attacking the problem. Because of the presence of the "extended source" parameter k_1 in the analytic program it was necessary to have some check on the analytic calculations. Although not as necessary, it was certainly as desirable to have an independent check on the Monte Carlo simulation. The curves were plotted on a Hewlett-Packard Calculator Plotter, Model 9125A, driven by an H-P Calculator, Model 9100A. The analytic curves are exact and the Monte Carlo curves are fit with an exponential regression program to the individual points obtained from the Monte Carlo computer runs. It is felt

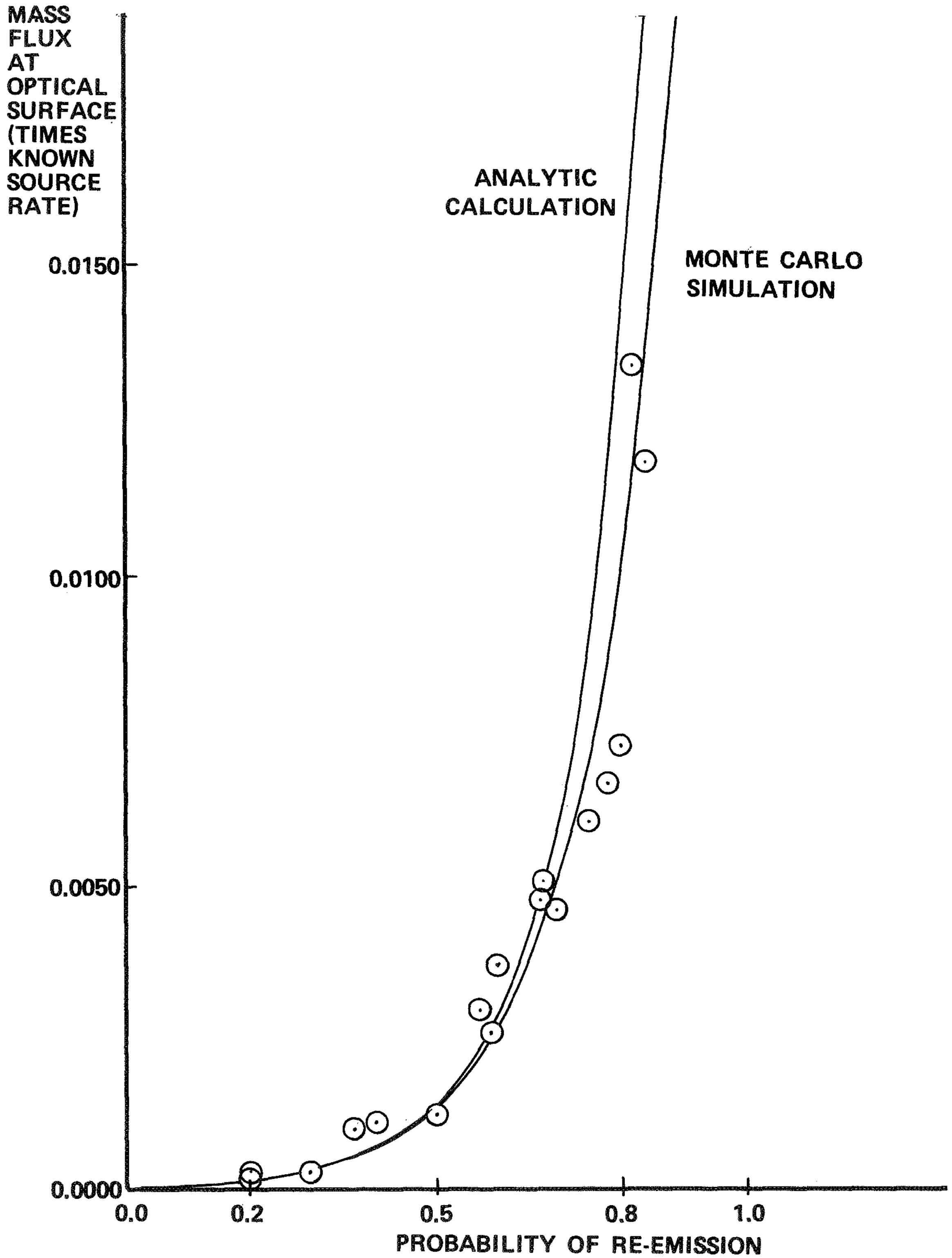


Figure 16. Sample calculations of top wall contribution to mass flux at optical surface.

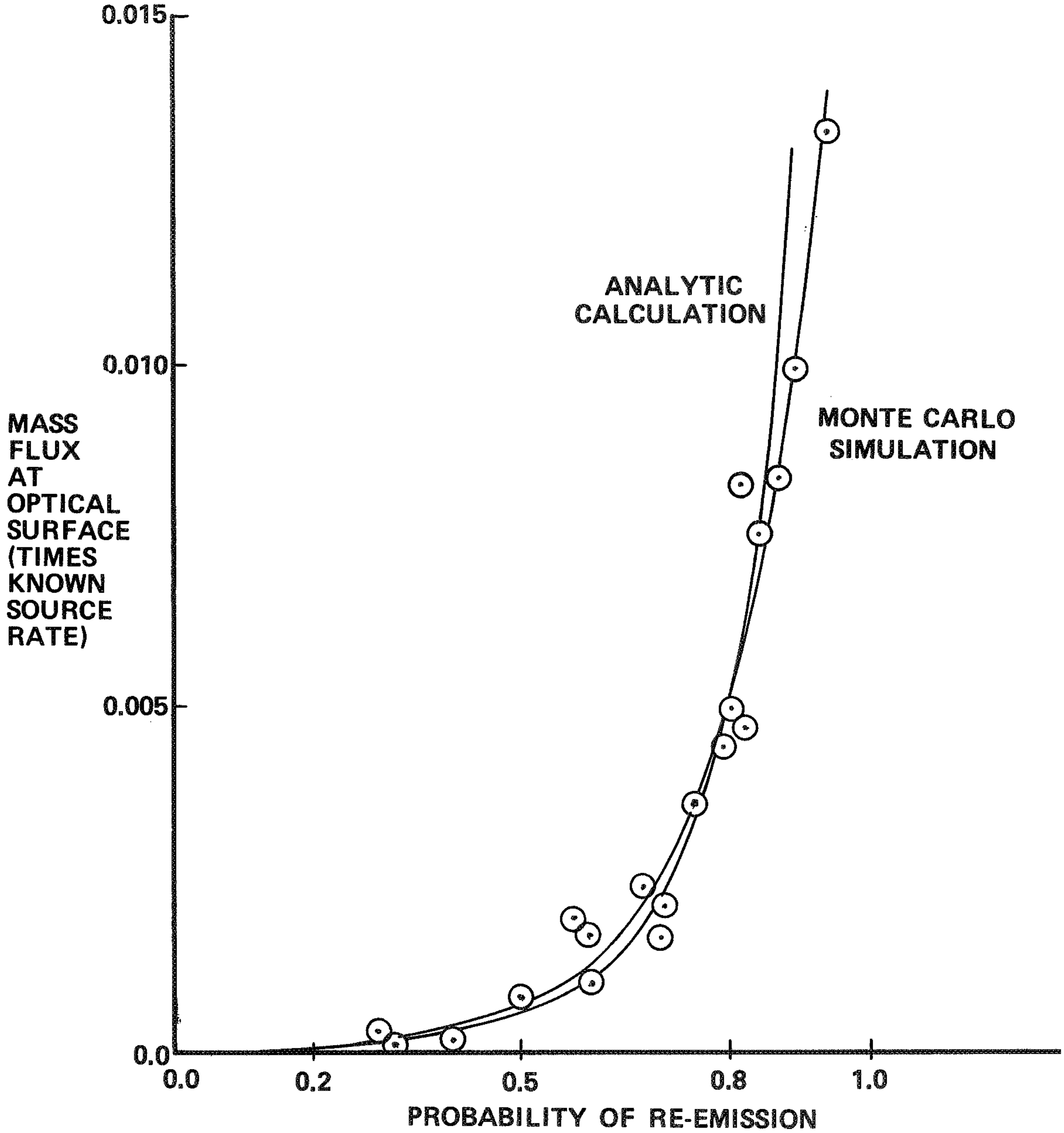


Figure 17. Sample calculations of back wall contribution to mass flux at optical surface.

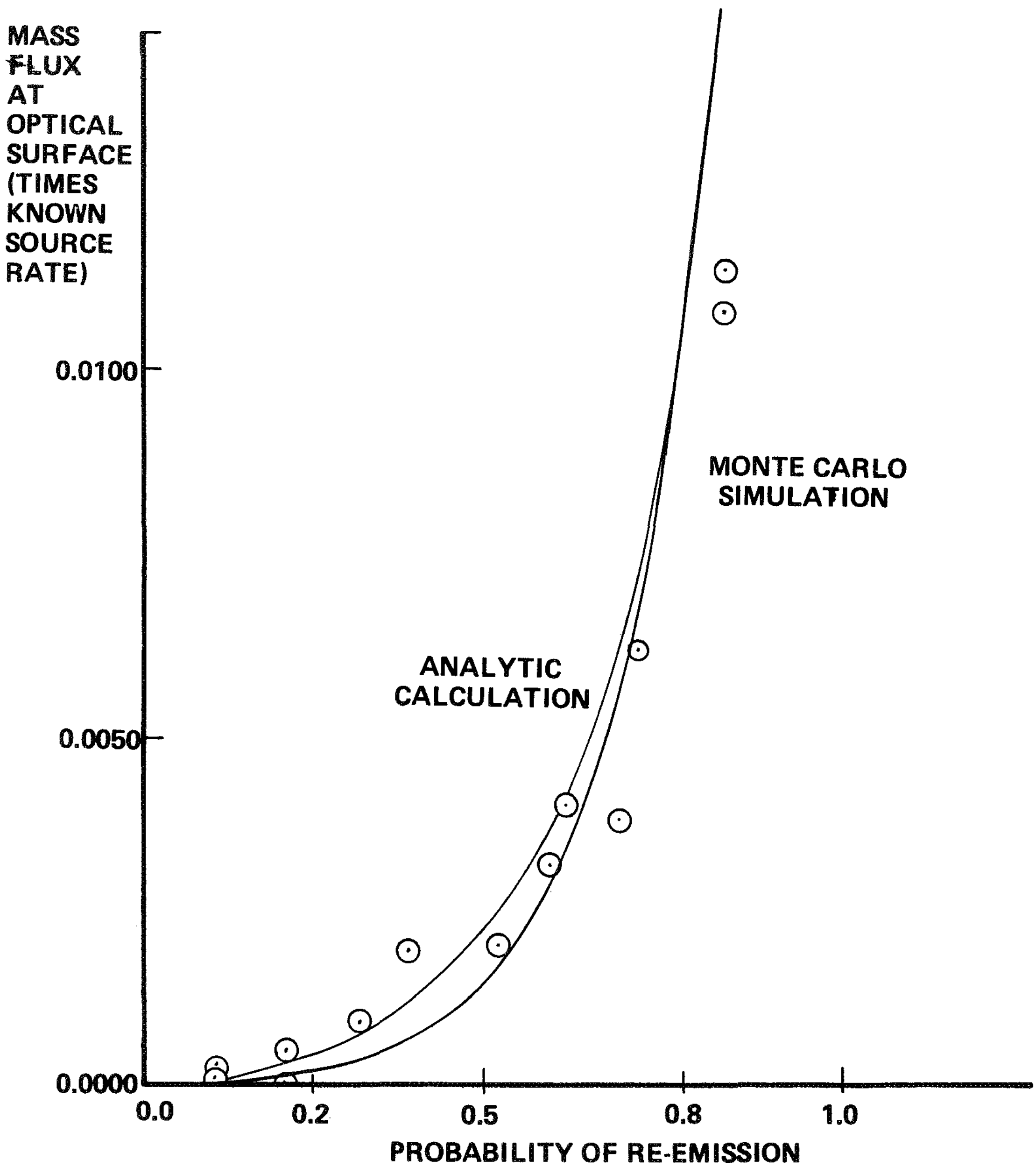


Figure 18. Sample calculations of bottom wall contribution to mass flux at optical surface.

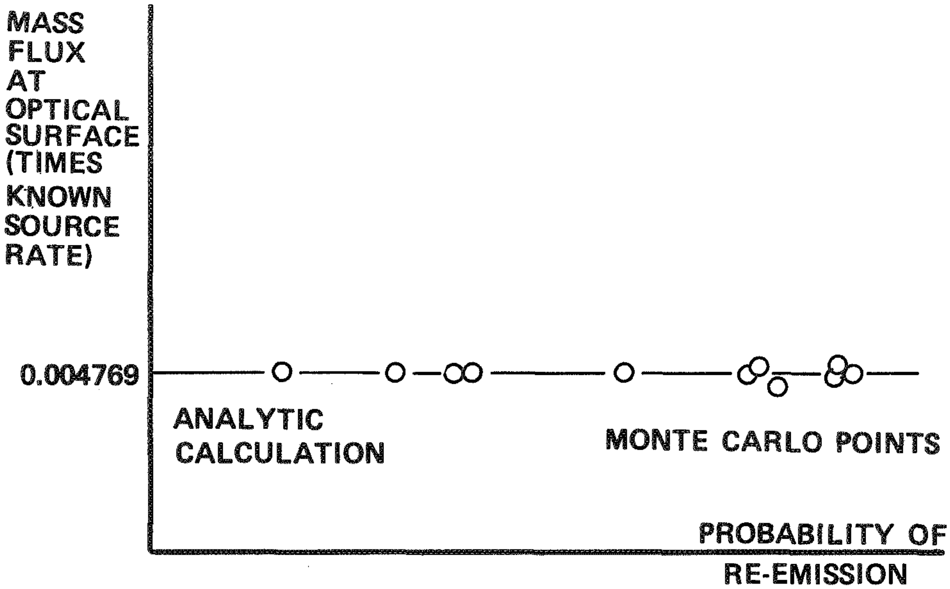


Figure 19. Sample calculations of those hits going from source directly to optical surface.

that the remarkable agreement between two such dissimilar methods of solving the problem is sufficient to allow the conclusion that the Monte Carlo method has been proven successful in its application. Such a conclusion is almost required before the much more complicated three-dimensional Monte-Carlo simulation is attempted.

It should also be pointed out here that with slight modifications the two-dimensional program can be used as an integral part of an experimental program to determine actual sticking coefficients.

The graphs (Figs. 16 through 19) are plotted such that the ordinate is always mass flux incident at the optical surface (times the known source rate) and the abscissa is the probability of re-emission from the walls. This parameter serves as the independent variable with mass flux dependent upon its value. Each wall is considered separately. It was not felt worth the effort to sum all the walls and compare the total flux, although this is one of the outputs of the Monte Carlo program. It should be mentioned that the contribution of those particles going directly from the source to the optical surface should be determined by the geometry and should obviously be independent of the probability of re-emission. This is seen to be the case in the relevant graph.

The computer program for the Monte Carlo calculation is listed in the appendix. The language is Fortran IV and the program was run on an IBM 1130.

APPENDIX

COMPUTER PROGRAM FOR THE MONTE CARLO CALCULATIONS

```
*EXTENDED PRECISION
      READ(2,170) XONE,YONE,XZERO,YZERO,YTOP,YBOT
  170 FORMAT(6F10.4)
C     INITIALIZE CONSTANTS
      ALPHI = 0.0
      BETAI = 0.0
C     DETERMINE WHICH WALL SOURCE IS ON AND DENOTE BY Q....... IF THE
C     SOURCE IS NOT ON ANY WALL THEN Q = 0 .... AFTER DETERMINATION IS
C     MADE THE QUADRANT ANGLES ARE CALCULATED
      IF(XZERO)2,1,2
    1 Q=1
      ALPHI =  QTAN(-XONE,YONE)
      BETAI=  QTAN(-XONE,YZERO)
      GO TO 10
    2 IF(YONE)4,3,4
    3 Q=2
      ALPHI =  QTAN(YZERO,XONE)
      BETAI=  QTAN(YZERO,XZERO)
      GO TO 10
    4 IF(XONE)6,5,6
    5 Q=3
      ALPHI  =   QTAN(XZERO,YZERO)
      BETAI =   QTAN(XZERO,YONE)
      GO TO 10
    6 IF (YZERO) 8,7,8
    7 Q = 4.
      ALPHI =  QTAN(YONE,XZERO)
      BETAI=  QTAN(YONE,XONE)
      GO TO 10
    8 Q=0
      AONE=  QTAN(YONE,XZERO)
      ATWO=  QTAN(YONE,XONE)
      ATHRE =  QTAN(YZERO,XONE)
      AFOUR=  QTAN(YZERO,XZERO)
      GO TO 10
   10 QSTAR =Q
      XL=XZERO-XONE
      YL=YONE-YZERO
C     DO DIFFERENT VALUES OF PSTIK USING K IF DESIRED
11    DO 96 K=3,4
      WRITE (3,777)
  777 FORMAT('   PSTIK      J        L     DIRECT     TOP    BACK     BOTTOM')
      PSTIK=1.2-.1*K
C     INITIALIZE THE COUNTERS
      ISUM=0
      L=1
      LZERO = 0
      LTWO = 0
      LTHRE = 0
      LFOUR = 0
```

```
C       INITIALIZE THE RANDOM NUMBER GENERATOR
        P = .1832*K/2.0
        T = .4621*K/2.0
        S = .6771*K/2.0
        R = .3473*K/2.0
    12 DO95 J = 1,10000
C       RUN  J-MAX PARTICLES WHERE J-MAX IS  END OF J DO-LOOP
C       RE-SET COLLISION COUNT TO ZERO
6200    I=0
C       RE-SET CO-ORDINATES TO ZERO FOR EACH NEW PARTICLE
        X=0.0
        Y=0.0
        ALPHA=ALPHI
        BETA=BETAI
        Q=QSTAR
C       CHECK THE COLLISION COUNT TO DETERMINE WHETHER THIS IS NEW
C       PARTICLE WITH RANDOM DISTRIBUTION OR COMING OFF A WALL WITH
C       COSINE DISTRIBUTION(UNLESS SOURCE IS ON WALL.. ...IF SO THE
C       IF TEST IN STATEMENT 16 WILL GIVE COSINE DIST ANYWAY)
    14 IF(I)99,16,90
    16 IF(Q)99,30,90
C       GENERATE RANDOM DISTRIBUTION ZERO TO TWO PI
30      CALL RANDN(R)
        ARGI=6.2831853*R
C       DETERMINE WHICH WALL THE PARTICLE HIT
    32 IF(AONE-ARGI)50,97,80
    50 IF(ATWO-ARGI)60,97,51
51      X=YONE /TAN(ARGI)
        GO TO 200
    60 IF(ATHRE -ARGI)70,97,61
    61 Y=XONE*TAN(ARGI)
        GO TO 300
    70 IF(AFOUR-ARGI)80,97,71
71      X=YZERO/TAN(ARGI)
        GO TO 400
    80 Y=XZERO*TAN(ARGI)
        GO TO 100
C       CHECK TO SEE WHETHER PARTICLE HIT THE LENS  .... IF IT DID THEN
C       GO TO ORIGIN AND START NEW PARTICLE RUN (INCREMENTING
C       COUNTERS AS THIS IS DONE)... IF NOT ,GENERATE NEW PROBABILITY
C       THAT PARTICLE WILL GET OFF OF WALL AND COMPARE WITH PSTIK
   100 IF(Y-YBOT )105,101,101
   101 IF(Y-YTOP)102,102,105
   102 L=L+1
        ISUM = ISUM + I
```

```
      WRITE(3,666) PSTIK,J,L,LZERO,LTWO,LTHRE,LFOUR
  666 FORMAT(2X,F6.3,6(2X,I5))
      IF(Q)99,103,104
  103 LZERO = LZERO+1
      GO TO 95
  104 IF(Q-2)99,702,106
  702 LTWO = LTWO+1
      GO TO 95
  106 IF(Q-3)99,704,107
  704 LTHRE = LTHRE+1
      GO TO 95
  107 IF(Q-4)99,706,99
  706 LFOUR = LFOUR+1
      GO TO 95
105   CALL RANDN(P)
      IF(P-PSTIK)95,108,108
C     DENOTE WALL HIT AND GENERATE QUADRANT ANGLES
  108 Q=1
      ALPHA=  QTAN(XL, YONE-Y )
      BETA=  QTAN(XL, YZERO-Y )
      GO TO 500
200   CALL RANDN(P)
      IF(P-PSTIK) 95,201,201
  201 Q=2
      ALPHA =   QTAN(YL, X-XONE )
      BETA =   QTAN(YL, X-XZERO )
      GO TO 500
300   CALL RANDN(P)
      IF(P-PSTIK) 95,301,301
  301 Q=3
      ALPHA=  QTAN( XL,Y-YZERO)
      BETA=  QTAN( XL,Y-YONE)
      GO TO 500
400   CALL RANDN(P)
      IF(P-PSTIK) 95,401,401
  401 Q=4
      ALPHA=  QTAN(YL, XZERO-X )
      BETA=  QTAN(YL,(XONE-X))
      GO TO 500
C     UPDATE COLLISION COUNTER
  500 I=I+1
      GO TO 14
```

```
C     GENERATE COSINE DISTRIBUTION ZERO TO PI
90    CALL RANDN(S)
      CALL RANDN(T)
      IF(T-S)85,85,86
   85 ARG=1.5707963*S
      GO TO 91
   86 ARG=3.141592*(1.0-T/2.0)
   91 IF(Q-1)99,110,92
C     DETERMINE FROM Q WHICH WALL WAS HIT AND CALCULATE THE POSITION
C     WHERE PARTICLE HIT
   92 IF(Q-2)99,210,93
   93 IF(Q-3)99,310,94
   94 IF(Q-4)99,410,99
  110 IF(ALPHA-ARG)120,97,111
  111 X=XZERO+(Y-YONE )*TAN(ARG)
      GO TO 200
  399 BETA = ARG
  120 IF(BETA-ARG)113,97,112
  112 Y=Y+XL/TAN(ARG)
      GO TO 300
  113 X=XZERO+(Y-YZERO)*TAN(ARG)
      GO TO 400
  210 IF(ALPHA-ARG)220,97,221
  221 Y=YONE+(XONE-X)*TAN(ARG)
      GO TO 300
  220 IF(BETA-ARG)223,97,222
  222 X=X-YL/TAN(ARG)
      GO TO 400
  223 Y=YONE+(XZERO-X)*TAN(ARG)
      GO TO 100
  310 IF(ALPHA-ARG)320,97,331
  331 X=XONE+(Y-YZERO)*TAN(ARG)
      GO TO 400
  320 IF(BETA-ARG)333,97,332
  332 Y=Y-XL/TAN(ARG)
      GO TO 100
  333 X=XONE+(Y-YONE)*TAN(ARG)
      GO TO 200
  410 IF(ALPHA-ARG)420,97,441
  441 Y=YZERO+(XZERO-X)*TAN(ARG)
      GO TO 100
  420 IF(BETA-ARG)443,97,442
  442 X=X+YL/TAN(ARG)
      GO TO 200
  443 Y=YZERO+(XONE-X)*TAN(ARG)
      GO TO 300
   97 WRITE(3,65)
   65 FORMAT('PARTICLE HAS HIT THE CORNER - RECYCLE.')
      GO TO 95
   99 WRITE(3,64)
   64 FORMAT('VARIABLE HAS IMPOSSIBLE VALUE.')
   95 CONTINUE
```

```
C     CALCULATE RATES FOR RUN JUST FINISHED
      RATE = FLOAT(L-1)/FLOAT(J)
      CAVG= FLOAT(ISUM)/FLOAT(L)
      DIRCT = FLOAT(LZERO)/FLOAT(J)
      WFOUR = FLOAT(LFOUR)/FLOAT(J)
      WTWO = FLOAT(LTWO)/FLOAT(J)
      WTHRE = FLOAT(LTHRE)/FLOAT(J)
C     PRINT OUT SUMMARY OF RUN FOR EACH VALUE OF PSTIK
      WRITE(3,701) J,PSTIK,CAVG,RATE,DIRCT,WTWO,WFOUR,WTHRE
  701 FORMAT(' SUMMARY OF ',I6,' PARTICLE RUN WITH PSTIK EQUAL ',F6.3
     1///' AVERAGE NUMBER OF COLLISIONS WITH THE WALLS WAS',F7.2///' THE
     2FLUX  RATE AT LENS FOR ALL PARTICLES WAS ',F8.5,' TIMES THE SOURCE
     3RATE.'//' THE DIRECT RATE FROM THE SOURCE WAS',F8.5//' THE RATE FR
     4OM THE TOP WALL WAS ',3X,F8.5/' THE RATE FROM THE BOTTOM WALL WAS'
     5F8.5/' THE RATE FROM THE BACK WALL WAS ',2X,F8.5)
   96 CONTINUE
   98 CONTINUE
      STOP
      END
```

```
      SUBROUTINE RANDN(Z)
      DATA I/1/
      REAL M
      IF(I) 1,2,1
1     I=0
      M=2.0**20
      X=566387.0
      A=2.0**10+3.0
2     X=A*X-IFIX(A*X/M)*M
      Z=X/M
      RETURN
      END
```

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2. Burrington, R.S.: Handbook of Mathematical Tables. Handbook Publishers, Inc. (Sandusky, Ohio), 1958.

APPROVAL

ANALYSIS OF A TWO-DIMENSIONAL MASS TRANSPORT PROBLEM CONTAMINATION OF SPACE FLIGHT EXPERIMENTS

By Edwin Klingman

The information in this report has been reviewed for security classification. Review of any information concerning Department of Defense or Atomic Energy Commission programs has been made by the MSFC Security Classification Officer. This report, in its entirety, has been determined to be unclassified.

This document has also been reviewed and approved for technical accuracy.

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