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ANNUAL REPORT

COOPERATIVE AGREEMENT NCC1-11

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Abstract

Remotely sensed optical data are now available to allow the characterization of phytoplankton from laser induced fluorescence of chlorophyll a. In this study, a radiative transfer computer model was developed to characterize the total flux of fluoresced or backscattered photons when laser radiation is incident on turbid water that contains a non-homogeneous suspension of inorganic sediments and phytoplankton. This radiative transfer model is based on the Monte Carlo technique. The computer model assumes that the aquatic medium can be represented by a stratified concentration profile and that appropriate optical parameters can be defined for each layer. The model is designed to minimize the required computer resources and run time. Results are presented for an anacystis marinus culture.

CONTENTS

The Monte Carlo Technique for Fluorescent Models

The Monte Carlo technique is based on the probabilities of occurrences of various events. Consider two possible physical events, "A" and "B", with relative probabilities of occurrences, P_A and P_B, respectively. If a random number, ϵ, is selected on the range 0 to 1 and ϵ is found to be less than P_A, then it can be assumed that event "A" occurred, otherwise event "B" occurred. In the Monte Carlo scheme, a process similar to this is repeatedly employed for any number of events until suitable statistics are achieved for the outcome. Thus a technique is available to predict the outcome of any definable sequence of events.

For the fluorescence of chlorophyll *a* in marine environments, a straight forward Monte Carlo approach can be used. A single photon of weight I_o is incident on the water surface at known azimuth and polar angles. Random numbers are selected to determine the course of events undertaken by the photon. Figure 1 shows the flow of possible events. In general, random numbers are selected to determine which of several events will be simulated and to select appropriate parameters via probability distribution functions. This latter technique is used to determine the distance a photon travels before some type of interaction occurs and the angles through which photons are scattered or fluoresced.

The photon's position must be continually monitored to determine if the water-air surface or other boundaries have been contacted. Whenever the photon leaves the medium, its position, direction of travel, wavelength and weight are recorded for further analysis.

Comparison With Other Techniques

There are several advantages in using the Monte Carlo technique for the laser induced fluorescence problem. First, any probability distribu-

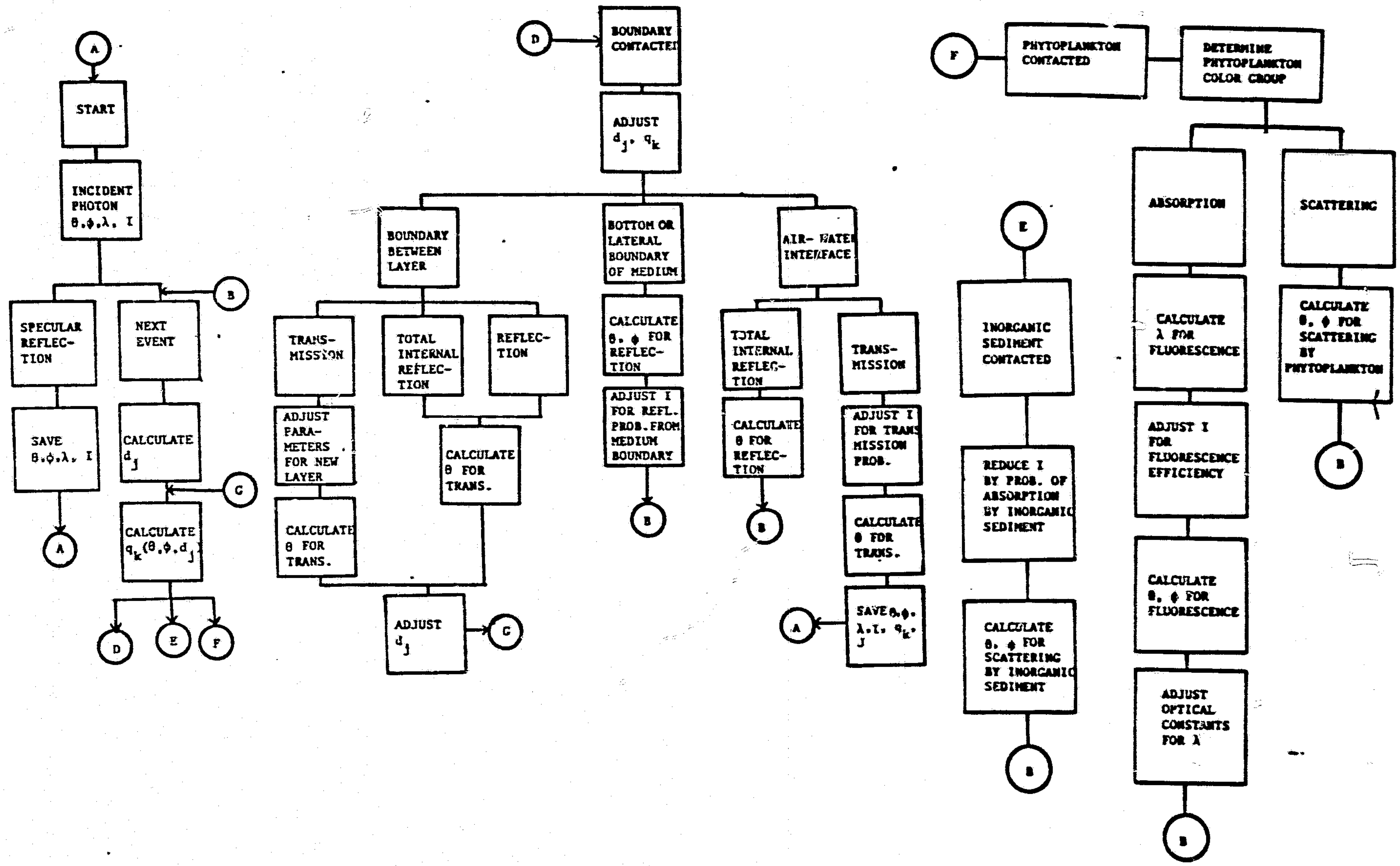
A
START
INCIDENT PHOTON θ,ϕ,λ, I
B
SPECULAR REFLEC-TION
NEXT EVENT
SAVE θ,ϕ,λ, I
CALCULATE d_j
C
A
CALCULATE $q_k(\theta,\phi,d_j)$
D
E
F
D
BOUNDARY CONTACTED
ADJUST d_j, q_k
BOUNDARY BETWEEN LAYER
BOTTOM OR LATERAL BOUNDARY OF MEDIUM
AIR- WATER INTERFACE
TRANS-MISSION
TOTAL INTERNAL REFLEC-TION
REFLEC-TION
ADJUST PARA-METERS FOR NEW LAYER
CALCULATE θ FOR TRANS.
CALCULATE θ FOR TRANS.
ADJUST d_j
C
CALCULATE θ, ϕ FOR REFLEC-TION
ADJUST I FOR REFL. PROB. FROM MEDIUM BOUNDARY
B
TOTAL INTERNAL REFLEC-TION
CALCULATE θ FOR REFLEC-TION
B
TRANS-MISSION
ADJUST I FOR TRANS MISSION PROB.
CALCULATE θ FOR TRANS.
SAVE θ, ϕ, λ, I, q_k, d_j
A
F
PHYTOPLANKTON CONTACTED
DETERMINE PHYTOPLANKTON COLOR GROUP
ABSORPTION
SCATTERING
CALCULATE λ FOR FLUORESCENCE
ADJUST I FOR FLUORESCENCE EFFICIENCY
CALCULATE θ, ϕ FOR FLUORESCENCE
ADJUST OPTICAL CONSTANTS FOR λ
B
CALCULATE θ, ϕ FOR SCATTERING BY PHYTOPLANKTON
B
E
INORGANIC SEDIMENT CONTACTED
REDUCE I BY PROB. OF ABSORPTION BY INORGANIC SEDIMENT
CALCULATE θ, ϕ FOR SCATTERING BY INORGANIC SEDIMENT
B

FIGURE 1

tion function can be used. Since we store these functions in tabular form, we can easily change from one function to another with a minimum of code changes. Second, the interaction medium can be easily divided into layers with different optical properties. The physical bounds of these layers can be easily changed. Finally, any number of detectors can be used simultaneously and various evaluation schemes can be used.

As with any technique there are some disadvantages. In general the technique may require large amounts of computer time. Statistical fluctuations might affect the results. Finally the method is impractical for extremely large optical depths.

Coordinate Transformation

The problems in coordinate translation and rotation have been solved in general (Kattawa). In our analysis we must keep track of the photons location at all times. In general, scattering angles are determined with respect to the photon's direction of travel prior to undergoing a scattering event. We must therefore determine the direction cosines of the new direction of travel with respect to a predefined fixed coordinate system. Some of the results derived here were presented by Kattawa.

A scattering event can be treated as a rotation of a coordinate system. See Figure 2. The vector, $\vec{P}_o$, represents the location of the photon prior to scattering. The z' axis of the rotated coordinated system is parallel with $\vec{P}_o$. The scattering polar, θ', and azimuth, ϕ', angles are defined with respect to the rotated (primed) coordinate system. Our task is to determine a set of direction cosines that defines the direction of travel of the photon after scattering with respect to the fixed coordinate system.

Vector $\vec{P}'$ represents the position of the photon after scattering. The components of $\vec{P}'$ in the rotated system are given by:

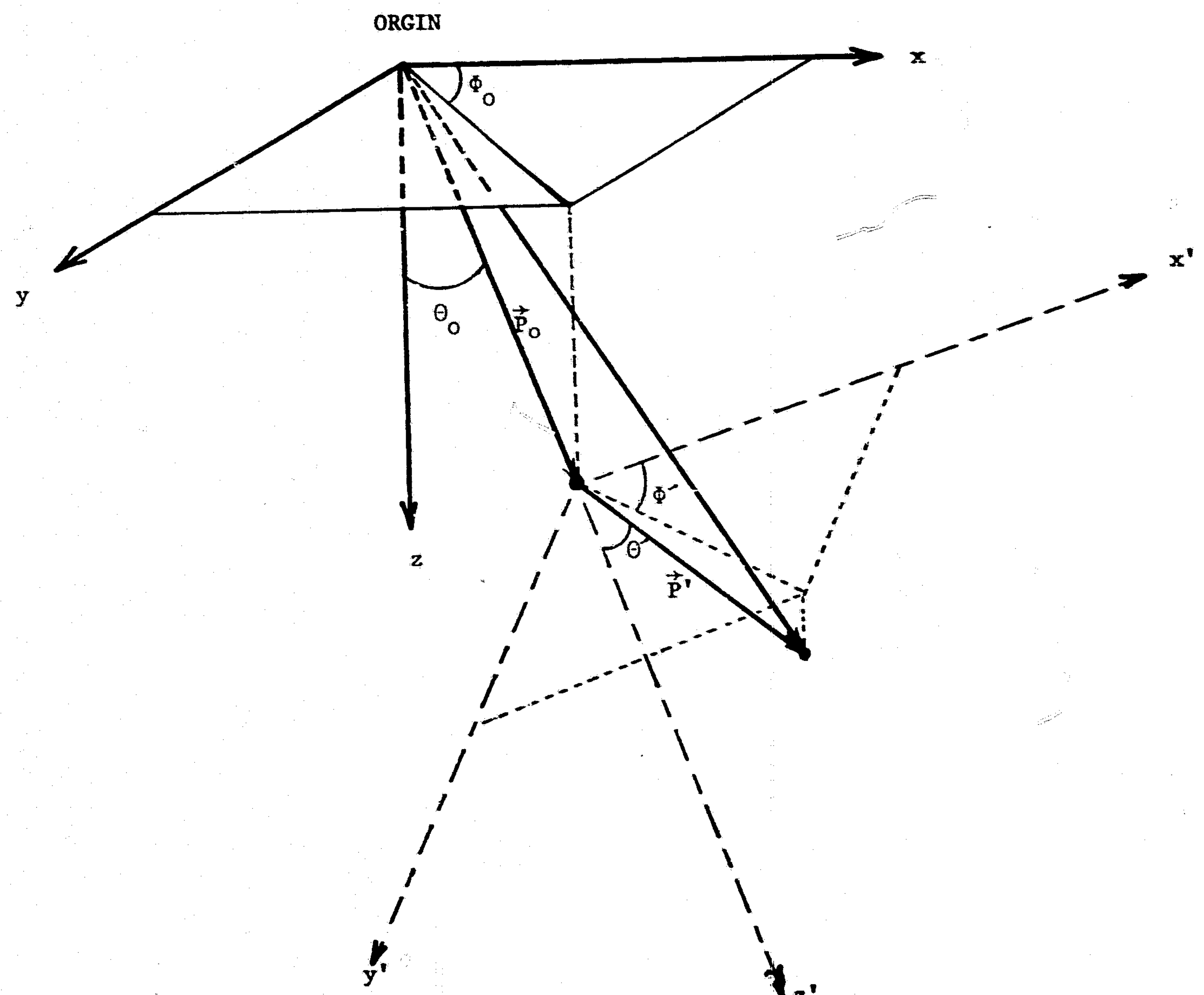

FIGURE 2

$$\vec{P}_x' = \hat{i}\, P'\sin\theta'\cos\phi' \tag{1a}$$

$$\vec{P}_y' = \hat{j}\, P'\sin\theta'\sin\phi' \tag{1b}$$

$$\vec{P}_z' = \hat{k}\, P'\cos\theta' \quad . \tag{1c}$$

The components of P′ in the fixed system are determined by two successive rotations. Let the polar and azimuthal angles in the fixed coordinate system before scattering be θ_o and ϕ_o respectively. Since the z′ axis is parallel to $\vec{P}_o$, these angles represent the degree of rotation between the two coordinate systems. First rotate through an angle ϕ_o about the z axis, resulting in an intermediate system, x", y", z". Next rotate through an angle θ_o about the y" axis. The resulting rotations are given by

$$\begin{bmatrix} P_x' \\ P_y' \\ P_z' \end{bmatrix} = \begin{bmatrix} \cos\theta_o & 0 & -\sin\theta_o \\ 0 & 1 & 0 \\ \sin\theta_o & 0 & \cos\theta_o \end{bmatrix} \begin{bmatrix} \cos\phi_o & \sin\phi_o & 0 \\ -\sin\phi_o & \cos\phi_o & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} P_x \\ P_y \\ P_z \end{bmatrix} \quad . \tag{2}$$

P_x, P_y, and P_z are the components of P in the fixed coordinate system, then

$$\begin{bmatrix} P_x \\ P_y \\ P_z \end{bmatrix} = M \begin{bmatrix} P_x' \\ P_y' \\ P_z' \end{bmatrix} \quad , \tag{3a}$$

where

$$M = \begin{bmatrix} \cos\theta_o\cos\phi_o & -\sin\phi_o & \sin\theta_o\cos\phi_o \\ \cos\theta_o\sin\phi_o & \cos\phi_o & \sin\theta_o\sin\phi_o \\ -\sin\theta_o & 0 & \cos\theta_o \end{bmatrix} \quad . \tag{3b}$$

Before scattering the direction cosines with respect to the fixed coordinate system are

$$u = \frac{P_{ox}}{P_o} = \sin\theta_o\cos\phi_o \tag{4a}$$

$$v = \frac{P_{oy}}{P_o} = \sin\theta_o\sin\phi_o \tag{4b}$$

$$w = \frac{P_{oz}}{P_o} = \cos\theta_o . \tag{4c}$$

Using equations (4a-c) and equation (3b) we have

$$\begin{bmatrix} P_x \\ P_y \\ P_z \end{bmatrix} = \begin{bmatrix} \frac{uw}{\sqrt{1-w^2}} & \frac{-v}{\sqrt{1-w^2}} & u \\ \frac{uw}{\sqrt{1-w^2}} & \frac{u}{\sqrt{1-w^2}} & v \\ -\sqrt{1-w^2} & 0 & w \end{bmatrix} \begin{bmatrix} BC \\ BD \\ A \end{bmatrix} \left| \vec{P}' \right| , \tag{5}$$

where $A = \cos\theta'$ (6a)

$B = \sin\theta'$ (6b)

$C = \cos\phi'$ (6c)

$D = \sin\phi'$. (6d)

Finally the direction cosines with respect to the fixed coordinate system are

$$\frac{P_x}{P'} = u' = \frac{uwBC-vBD}{\sqrt{1-w^2}} + uA \tag{7a}$$

$$\frac{P_y}{P'} = v' = \frac{vwBC+uBD}{\sqrt{1-w^2}} + vA \tag{7b}$$

$$\frac{P_z}{P'} = w' = -\sqrt{1-w^2}\,BC + wA \tag{7c}$$

For coordinate translation we have

$$P_x = P_{ox} + P'u' \tag{8a}$$

$$P_y = P_{oy} + P'v' \tag{8b}$$

$$P_z = P_{oz} + P'w' \quad . \tag{8c}$$

The series of equations derived above are used to determine the location of the photon after each event. If θ_o approaches 0, then equations (7a-c) must be modified. Then

$$u' = BCw \tag{8a}$$

$$v' = BD \tag{8b}$$

$$w' = Aw \quad . \tag{8c}$$

Step Profiles

A stratfied model is used to represent changes in optical parameters as a function of depth. This approach allows homogeneous layers of various thicknesses to represent changing concentration profiles. We assume that appropriate optical parameters can be defined for each layer. No lateral variations in optical parameters are allowed.

Special consideration must be given when the photon moves to the interface between two layers. Figure 3 depicts a case in which a photon starts in layer 1 and travels toward layer 2. We select the distance the photon travels, d_j, from an appropriate distribution function. The value of d_j is the distance the photon would travel in a homogeneous media, that is if it remained in layer 1. This distance does not account for optical properties of layer 2. When the trajectory reaches the interface several results are possible. If there is a difference in the refractive indices of the two layers, there will be a finite probability of reflection at the interface. We then compare a randomly selected number to the reflection

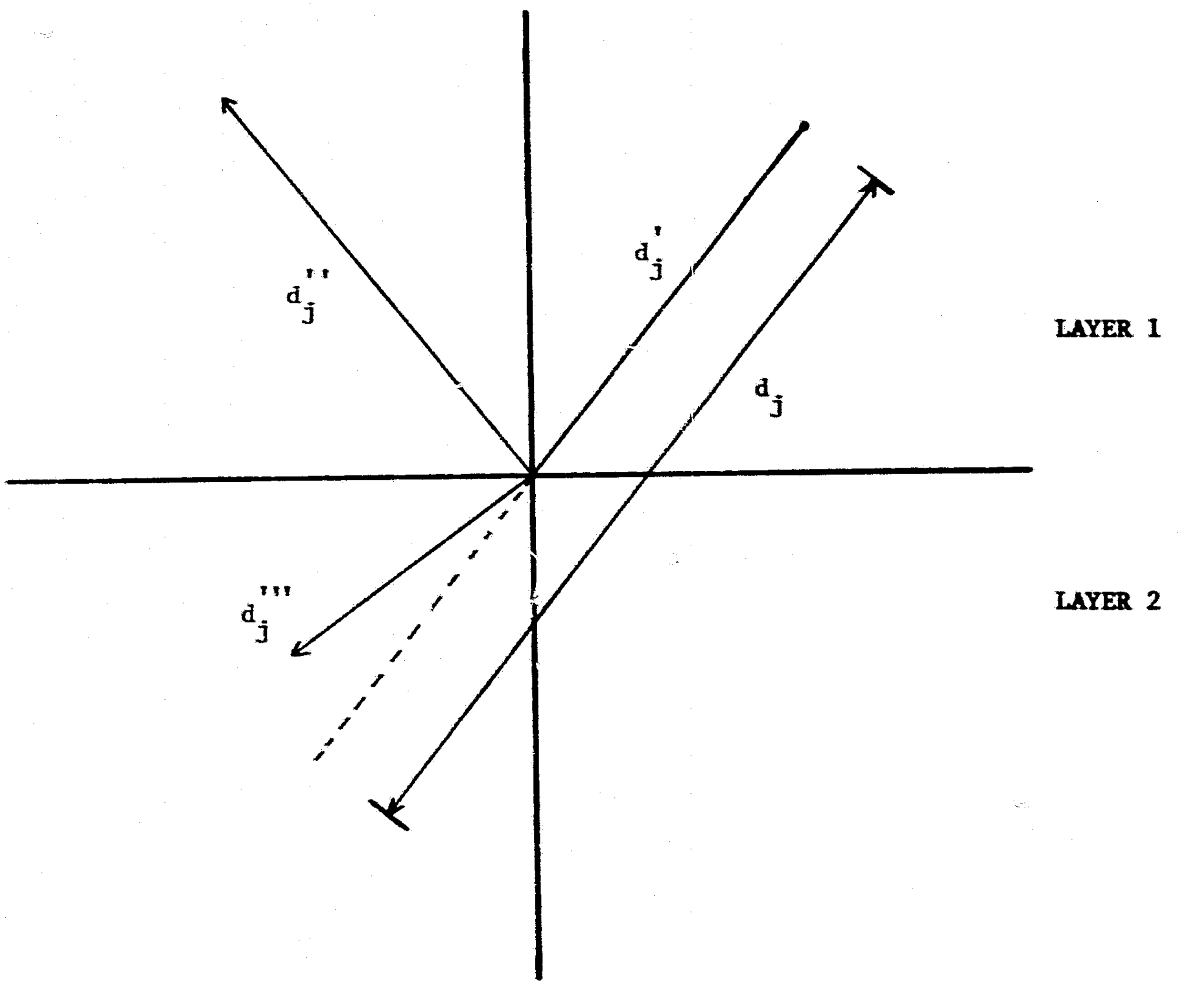

FIGURE 3

probability. If it is found that reflection is to be simulated the reflection angles are determined, the trajectory is adjusted for reflection at these angles and the photon continues its path in layer 1. Prior to reflection the photon travels a distance d_j' and after reflection the photon travels d_j'' such that

$$d_j' + d_j'' = d_j \qquad (9)$$

If the photon is not reflected at the interface, then refraction must be simulated. Appropriate refraction angles are calculated and the photon is made to enter layer 2. The distance that the photon travels in layer 2, d_j''', will depend on the relative optical attenuation coefficients of layers 1 and 2.

$$d_j''' = (d_j - d_j') \frac{\alpha_T^{(1)}}{\alpha_T^{(2)}} \qquad (10)$$

where $\alpha_T^{(i)}$ is the total optical attenuation coefficient of layer i.

<u>Distance to Vertical Bounds</u>

It is necessary to determine the distance from the photon to any vertical bound to ascertain if the photon reaches the boundary for a particular d_j value. Figure 4a is a horizontal projection of the photon's trajectory and a section of the cyclindrical vertical boundary; Figure 4b is the vertical projection. The photon is located at coordinate (x, y, z) and its new direction of travel is given by $\vec{d}_j$. R_o represents the horizontal distance from the origin to the photon and R_t is the horizontal distance from the origin to the point where the photon will intercept the boundary. Also, d_w is the distance from the photon to the boundary along the direction of travel and d is the horizontal projection of d_w. The angles α and β are respectively the angles that R_o and d make with the x axis and θ is the angle that d_w makes with the z axis. The distance d_w is related

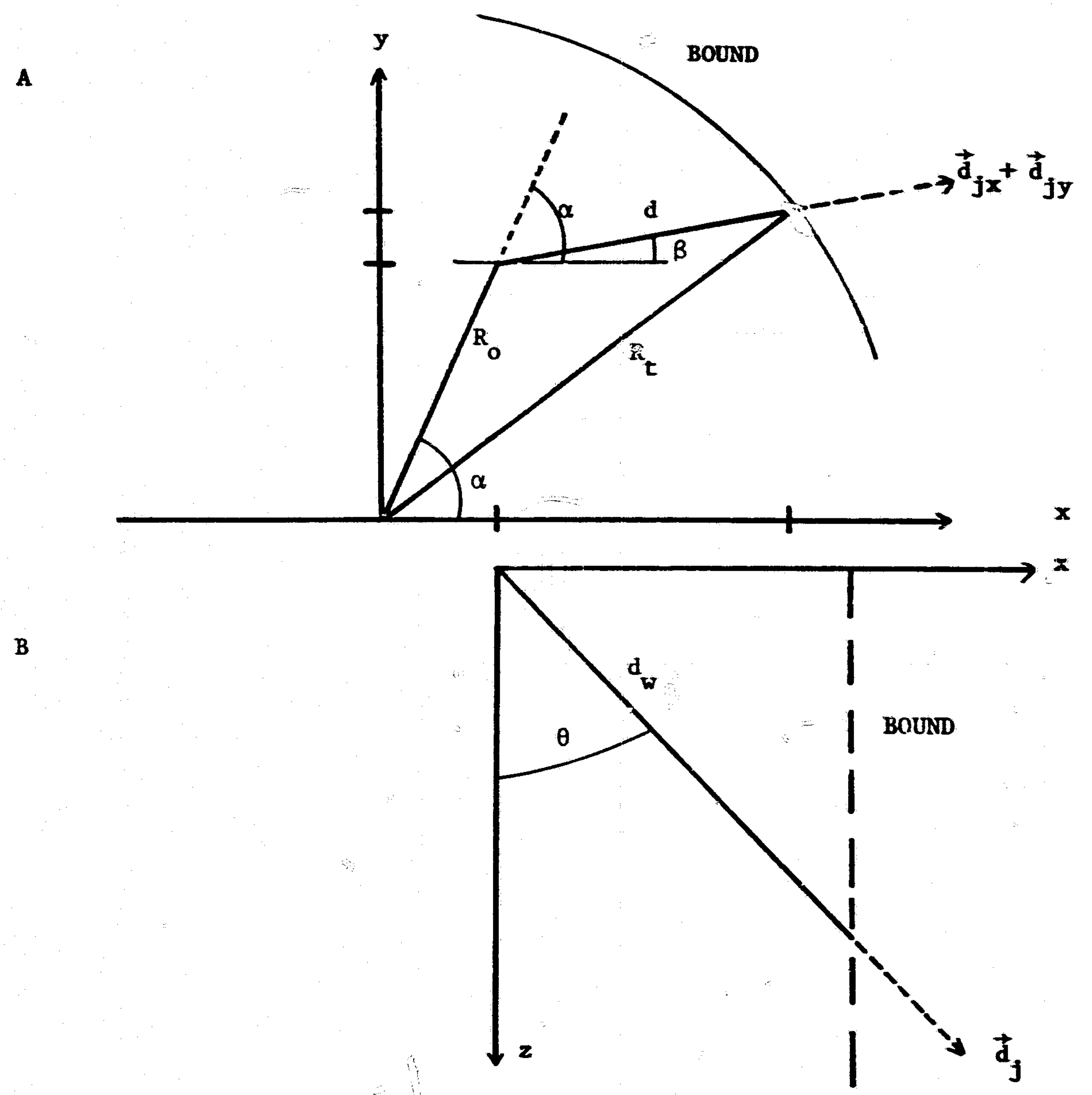
A
B
y
x
x
z
BOUND
BOUND
$\vec{d}_{jx} + \vec{d}_{jy}$
$\vec{d}_j$
d
β
α
α
R_o
R_t
d_w
θ

FIGURE 4

to d by the expression

$$d_w = \frac{d}{\sin\theta} \quad . \tag{11}$$

The direction cosines of d_w are

$$u = \cos\beta\sin\theta \tag{12}$$

$$v = \sin\beta\sin\theta \tag{13}$$

$$w = \cos\theta \quad . \tag{14}$$

The distance R_t is given by the relationship

$$R_t^{\,2} = R_o^{\,2} + d^2 + 2R_o d\ \cos(\alpha-\beta) \quad . \tag{15}$$

Using equations (12, 13 and 14) and a trigonometric identity, the $\cos(\alpha-\beta)$ can be written

$$\cos(\alpha-\beta) = \frac{x}{R_o}\ \frac{u}{\sin\theta} + \frac{y}{R_o}\ \frac{v}{\sin\theta} \quad . \tag{16}$$

Combining equations (16 and 15) and solving for d, we have

$$d = -\frac{xu+yv}{\sin\theta} + \sqrt{\left(\frac{xu+yv}{\sin\theta}\right)^2 + R_t^{\,2} - R_o^{\,2}} \tag{17}$$

and using equations (11) and (14), we have

$$d_w = -\frac{xu+yv}{1-w^2} + \frac{1}{\sqrt{1-w^2}}\sqrt{\frac{(xu+yv)^2}{1-w^2} + R_t^{\,2} - R_o^{\,2}} \quad . \tag{18}$$

Reflection at Vertical Bounds

If we determined that the photon reaches a vertical bound, it is forced to be reflected. The new direction of travel after reflection must be determined. Figure 5 shows the geometry for this task. When the photon is reflected from a vertical bound a rotated coordinate system is defined with its z' axis perpendicular to the boundary and its x' axis in the $-z$ direction. The new polar and azimuthal angles, θ' and ϕ', respectively, are defined with respect to the rotated system from appropriate distribution functions. We must again find the direction cosines with respect

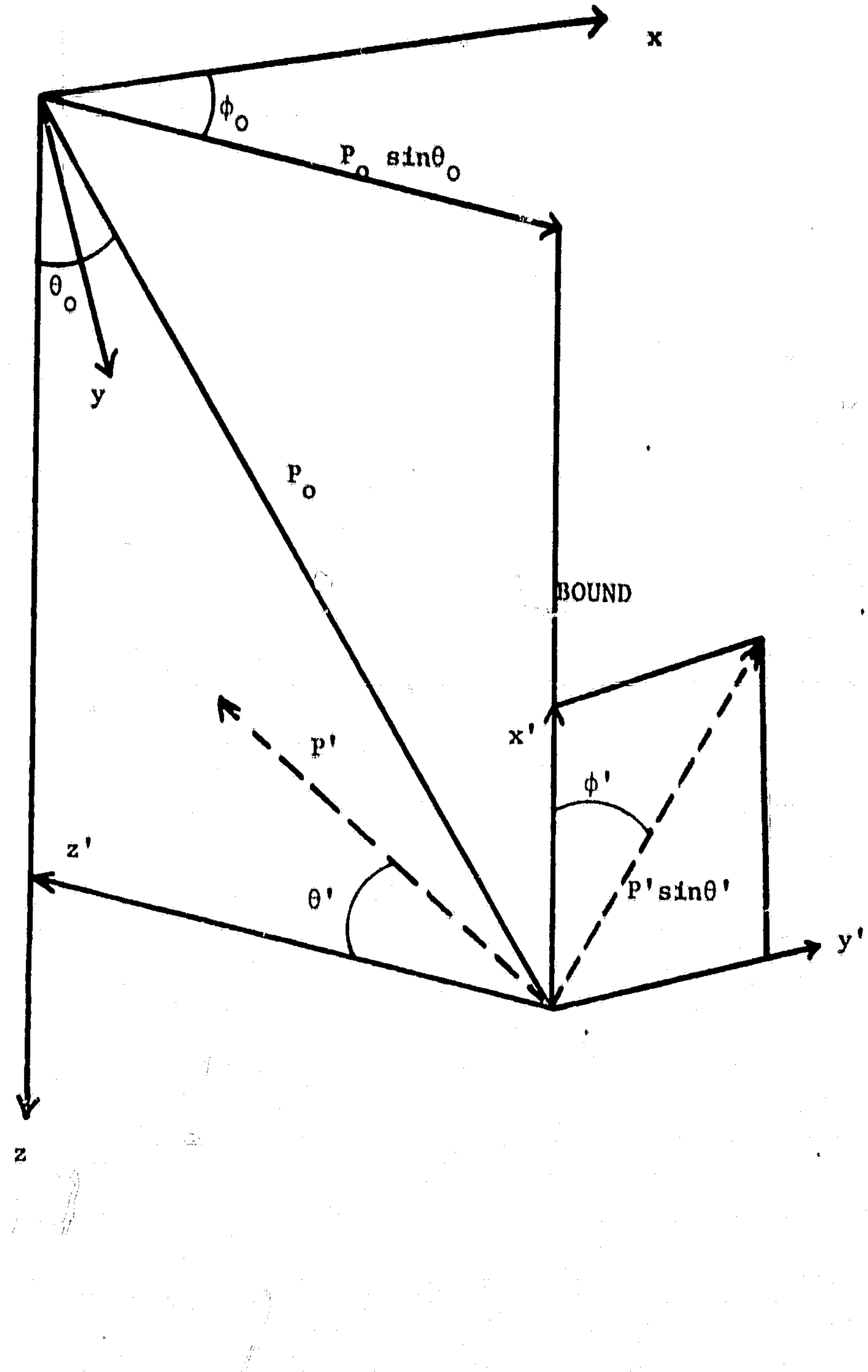
x
ϕ_o
$P_o \sin\theta_o$
θ_o
y
P_o
BOUND
x'
p'
ϕ'
z'
θ'
$P'\sin\theta'$
y'
z

FIGURE 5

to the fixed coordinate system.

To accomplish this we first rotate through an angle $-\pi/2$ about the y' axis. This aligns the z' and z axes. The rotation creates an intermediate coordinate system x'', y'', z''. We then rotate through an angle $\pi-\phi_o$ to align the x'' and x axes. Mathematically these rotations are represented as follows:

$$\begin{bmatrix} P_x \\ P_y \\ P_z \end{bmatrix} = \begin{bmatrix} \cos(\pi-\phi_o) & \sin(\pi-\phi_o) & 0 \\ -\sin(\pi-\phi_o) & \cos(\pi-\phi_o) & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \cos(-\pi/2) & 0 & -\sin(-\pi/2) \\ 0 & 1 & 0 \\ \sin(-\pi/2) & 0 & \cos(-\pi/2) \end{bmatrix} \begin{bmatrix} P_x' \\ P_y' \\ P_z' \end{bmatrix} \tag{19}$$

$$= M \begin{bmatrix} P_x' \\ P_y' \\ P_z' \end{bmatrix} , \tag{20}$$

where P' is the position vector of the photon after reflection in the rotated system and

$$M = \begin{bmatrix} 0 & \sin\phi_o & -\cos\phi_o \\ 0 & -\cos\phi_o & -\sin\phi_o \\ -1 & 0 & 0 \end{bmatrix} . \tag{21}$$

The direction cosines of z' (normal to the boundary) with respect to the fixed coordinates are determined by noting that z' is perpendicular to z. Thus

$$v = -\sin\phi_o \tag{22}$$

$$u = -\cos\phi_o \tag{23}$$

$$w = 0 . \tag{24}$$

The coordinates of the photon after reflection from the bound are

$$x' = P'\sin\theta' \cos\phi' = P'BC \tag{25}$$

$$y' = P'\sin\theta' \sin\phi' = P'BD \tag{26}$$

$$z' = P'\cos\theta' = P'A \ . \tag{27}$$

The direction cosines in the fixed coordinate system are then obtained from equation (20, 22-24 and 25-27).

$$u' = \frac{x'}{P'} = -uBD+uA \tag{28}$$

$$v' = \frac{y'}{P'} = uBD+vA \tag{29}$$

$$w' = \frac{z'}{P'} = -BC \ . \tag{30}$$

It should be noted that equations (28-30) can also be obtained by substituting equation (24) into equations (7a-7c).

Distance to Horizontal Boundaries

We now develop an equation that determines the distance to a horizontal bound. See Figure 6. The distance, along the direction of travel, from the present location of the photon x, y, z to a horizontal bound is given by

$$d_H = \frac{d_T - z}{\cos\theta} = \frac{d_T - z}{w} \ . \tag{31}$$

Here θ is the angle between the direction of travel and the z axis of the fixed coordinate system and d_T is the thickness of the horizontal layer.

Reflection of Horizontal Bounds

Two types of reflections occur at horizontal boundaries. Specular reflection occurs at the air water interface and at layer boundaries. Non-specular reflection occurs at the bottom surface layer, for example the ground or tank bottom.

When a photon is reflected nonspecularly, a new coordinate system is defined with the z′ axis normal to the lower surface (anti-parallel to

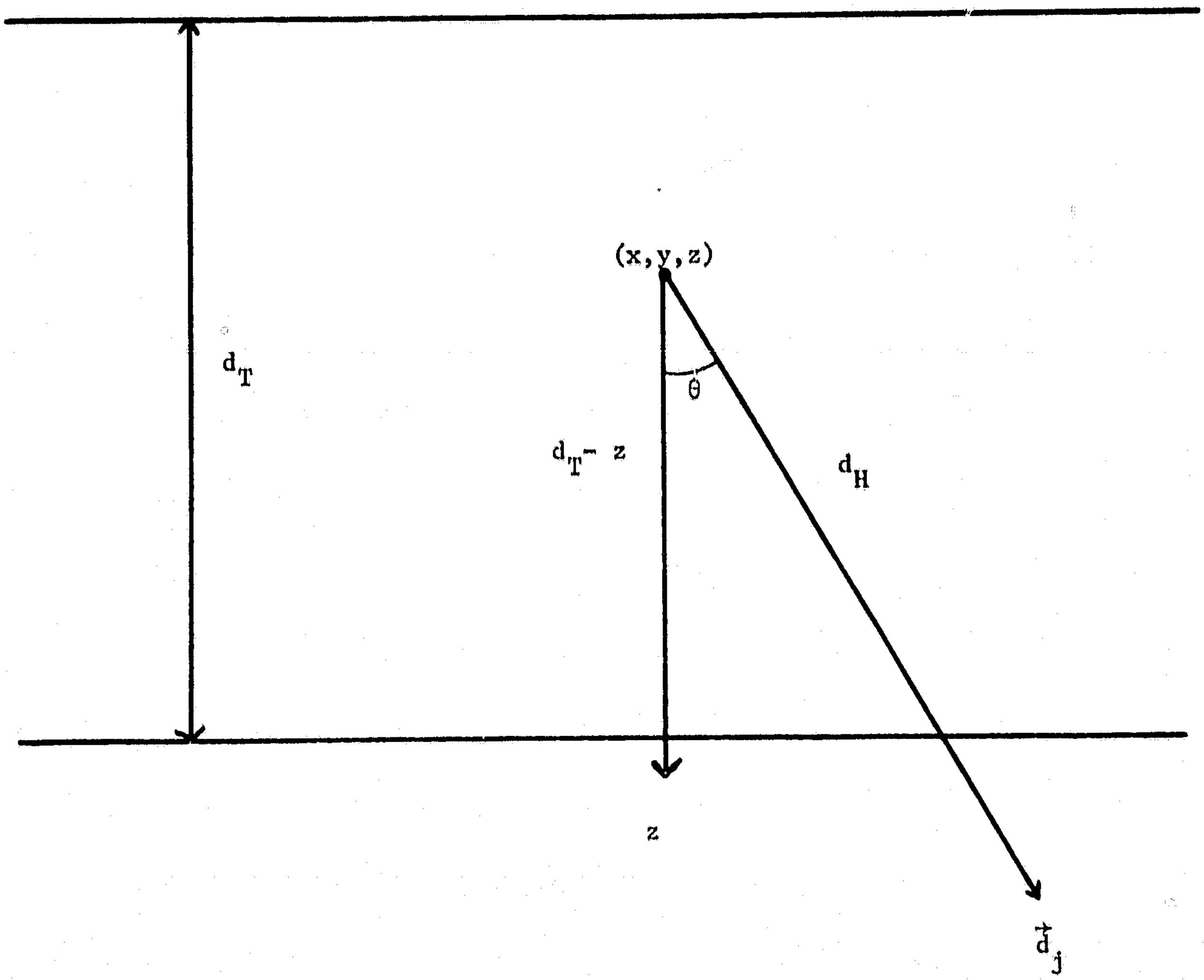

FIGURE 6

the z axis) and the y' axis is defined to be paralled to the y axis, see Figure 7. The angles through which the photon is reflected, θ' and ϕ', are defined with respect to the new coordinate system. These angles are selected from an appropriate distribution function. A single rotation through an angle of π about the y' axis will align the coordinate systems. The position vector, $\vec{P}'$ has components

$$P_x' = P'\sin\theta'\cos\phi' = P'BC \tag{32}$$

$$P_y' = P'\sin\theta'\sin\phi' = P'BD \tag{33}$$

$$P_z' = P'\cos\theta' \quad = P'A. \tag{34}$$

The components of $\vec{P}'$ in the fixed coordinate system are given by

$$\begin{bmatrix} P_x \\ P_y \\ P_z \end{bmatrix} = \begin{bmatrix} \cos\pi & 0 & -\sin\pi \\ 0 & 1 & 0 \\ \sin\pi & 0 & \cos\pi \end{bmatrix} \begin{bmatrix} P_x' \\ P_y' \\ P_z' \end{bmatrix} . \tag{35}$$

Thus the direction cosines of P in the fixed coordinate system are

$$u' = -BC \tag{36}$$

$$v' = \ \ BD \tag{37}$$

$$w' = -A \tag{38}$$

For specular reflection, the angle of incidence is equal to the angle of reflection when measured with respect to a normal to the surface. Thus the polar angle after reflection θ' is related to the polar angle before reflection, θ_o by the relationship

$$\theta' = \pi-\theta_o. \tag{39}$$

Since specular reflection does not change the photon's plane of motion, the azimuthal angle does not change,

$$\phi' = \phi_o. \tag{40}$$

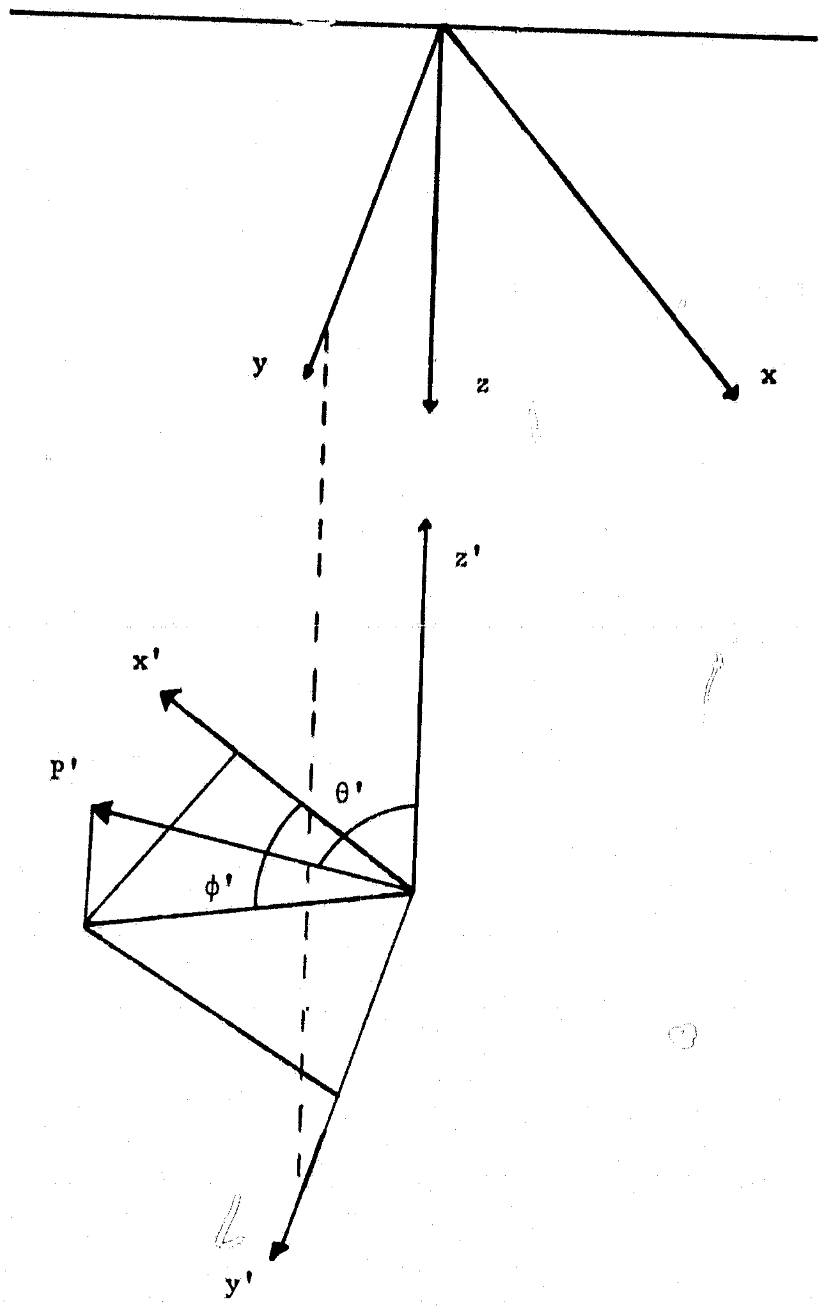

FIGURE 7

The new direction cosines are thus

$$u' = u \tag{41}$$

$$v' = v \tag{42}$$

$$w' = w \ . \tag{43}$$

Refraction at Horizontal Surfaces

For refraction, the photon travels from one transparent medium of refractive index, r_o, to a medium of different refractive index, r'. The azimuthal angle does not change upon refraction. The polar angle changes in accordance with Snell's Law of Refraction

$$r_o \sin\theta_o = r' \sin\theta \ . \tag{44}$$

The initial direction cosines of the photon's position vector, $\vec{P}_o$, are

$$u = \sin\theta_o \cos\phi_o \tag{45}$$

$$v = \sin\theta_o \sin\phi_o \tag{46}$$

$$w = \cos\theta_o . \tag{47}$$

The direction cosines after refraction can be calculated from equation (44) and equations (45-47).

$$u' = \sin\theta' \cos\phi' = \frac{r_o}{r'} \sin\theta_o \cos\phi_o \tag{48}$$

$$v' = \sin\theta' \sin\phi' = \frac{r_o}{r'} \sin\theta_o \sin\phi_o \tag{49}$$

$$w' = \cos\theta' = \sqrt{1-\left(\frac{r_o}{r'}\right)^2 \sin^2\theta_o} . \tag{50}$$

These equations can be written in terms of the initial direction cosines.

$$u' = \frac{r_o}{r'} u \tag{51}$$

$$v' = \frac{r_o}{r'} v \tag{52}$$

$$w' = \sqrt{1-\left(\frac{r_o}{r'}\right)^2 \left(1-w^2\right)} \tag{53}$$

Reflection Coefficients

Fresnel reflection probabilities are used to determine if the photon is to be reflected or transmitted. Since we have developed our coordinate transformations in terms of direction cosines, it is convenient to express the Fresnel reflection coefficient in a similar manner. If the photon makes an angle θ_o with the z axis before refraction and an angle θ' with this axis after refraction, the Fresnel reflection coefficient, f_r, is then

$$f_r = \frac{1}{2}\left[\frac{\tan^2(\theta'-\theta_o)}{\tan^2(\theta'+\theta_o)} + \frac{\sin^2(\theta'-\theta_o)}{\sin^2(\theta+\theta_o)}\right]. \tag{54}$$

Writing the tangent function in terms of sine and cosine functions and using equations (47) and (53), equation (54) can be written

$$f_r = \frac{1}{2}\left[\frac{\frac{r_o}{r'} w-w'}{\frac{r_o}{r'} w+w'}\right]^2 \left[1 + \left[\frac{ww' - \frac{r_o}{r'} (1-w^2)}{ww' + \frac{r_o}{r'} (1-w^2)}\right]\right] . \tag{55}$$

Optical Parameters

The radiative transfer is influenced by the optical properties of the medium. In general a total attenuation coefficient can be defined for a homogeneous medium. Several concerns exist: scattering and absorption for pure water, scattering and absorption for suspended passive particulates, and scattering and absorption for chlorophyll a. If photons are absorbed by chlorophyll, then fluorescence must be considered. The total attenuation at wavelength, λ, of the medium can be represented by

$$\alpha_T(\lambda) = \alpha_w(\lambda) + \alpha_p(\lambda) + \alpha_c(\lambda) \tag{56}$$

where $\alpha_w(\lambda)$, $\alpha_p(\lambda)$ and $\alpha_c(\lambda)$ are the total attenuation coefficients for water, suspended particulates and chlorophyll a, respectively. Each attenuation coefficient can be written in terms of a scattering coefficient, s, and an absorption coefficient, a,

$$\alpha_w(\lambda) = a_w(\lambda) + s_w(\lambda) \tag{57}$$

$$\alpha_p(\lambda) = a_p(\lambda) + s_p(\lambda) \tag{58}$$

$$\alpha_c(\lambda) = a_c(\lambda) + s_c(\lambda). \tag{59}$$

Again the subscripts w, p, and c corresponds to water, particulates and chlorophyll a.

Scattering

For our simulations, it is assumed that scattering by pure water is negligible. When it is decided that a scattering event by phytoplankton or particulates is to be simulated, it becomes necessary to determine the direction of travel of the photon after scattering. An appropriate scattering phase function must be used. A typical function for polar angles is shown in Figure 9. These data are stored in the computer in tabular

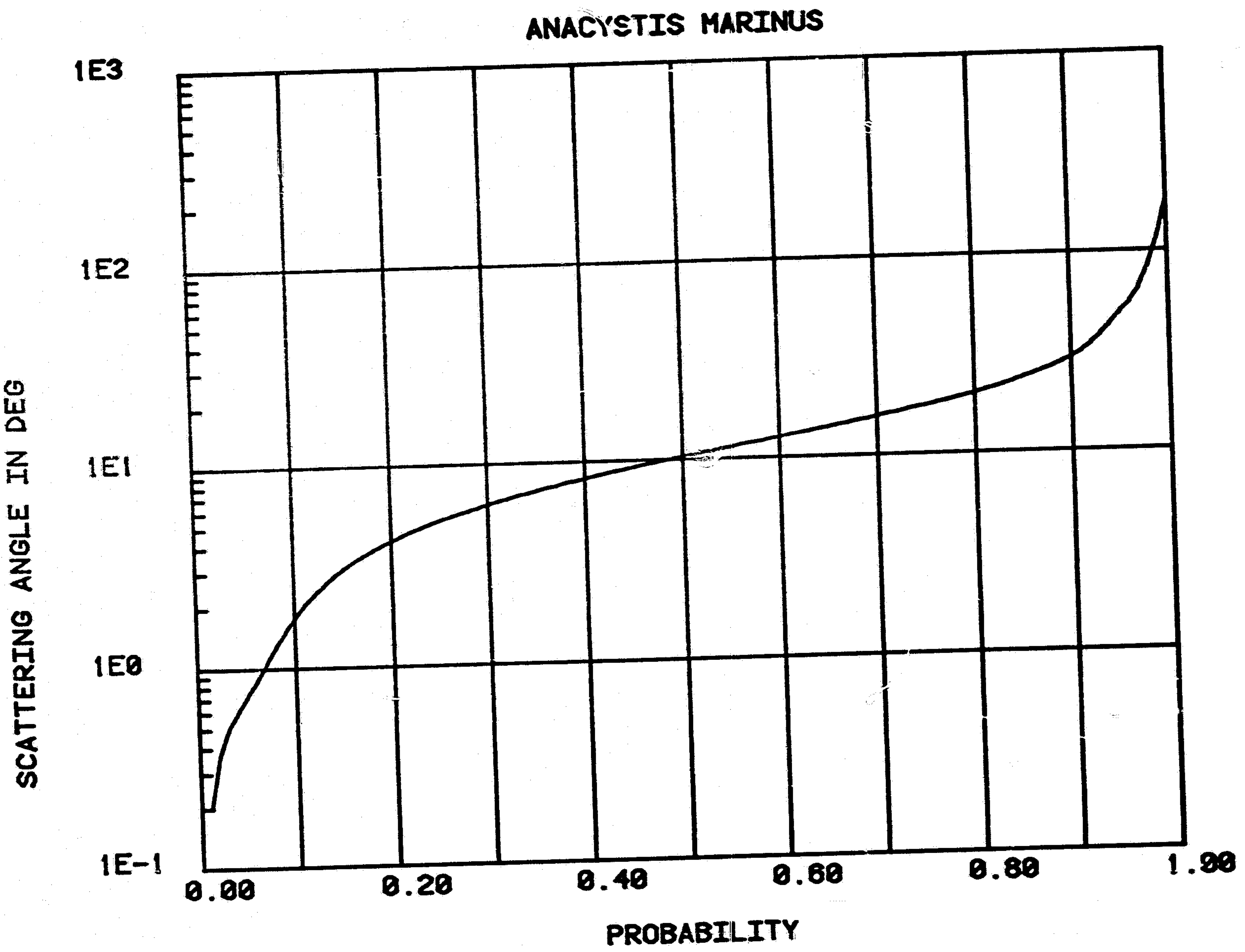
ANACYSTIS MARINUS
1E3
1E2
1E1
1E0
1E-1
SCATTERING ANGLE IN DEG
0.00
0.20
0.40
0.60
0.80
1.00
PROBABILITY

FIGURE 9

form and the appropriate polar angle is determined by selecting a random number, ε, and comparing this number to the probability of scattering at a particular angle. For example, if $\varepsilon = 0.1$, then from Figure 9, the appropriate polar scattering angle will be 1.1 degrees.

The azimuthal angle is assumed to be evenly distributed on the range $-\pi$ to π and can thus be randomly selected by the function

$$\phi' = \pi(2\varepsilon-1),\ 0< \varepsilon <1. \tag{60}$$

Since scattering can also occur on contact with vertical and horizontal bounds, appropriate scattering functions must be defined for these situations. For these cases, we assume Lambertian surfaces which produce the same luminance in all outward directions (Driscoll). It is thus assumed that the $\sin^2\theta'$ is evenly distributed on the range 0 to 1, and ϕ' is evenly distributed from $-\pi$ to π. In terms of randomly selected numbers θ' and ϕ' for reflection from Lambertian surfaces are defined by the equations

$$\sin\theta' = \sqrt{\varepsilon_1} \tag{61}$$

$$\cos\theta' = \sqrt{1-\varepsilon_1} \tag{62}$$

$$\phi' = \pi(2\varepsilon_2-1). \tag{63}$$

Absorption

In all cases appropriate absorption coefficients are needed for water. For our simulations, we use the values reported in the literature (Smith and Taylor). The effects of pure water absorption are accounted for by adjusting the weight of the photon each time a trajectory of length d_j is traversed. If I_o is the initial weight of the photon, the adjusted weight due to water absorption is

$$I_o'' = I_o e^{-a_w(\lambda)d_j} \tag{64}$$

If a suspended particulate is contacted, the absorption is again accounted for by a weight adjustment. The procedure we follow in this case is to force a scattering process and reduce the weight of the photon by the relative probability that scattering would have occurred. (See Appendix 1). The photon's weight after scattering is then

$$I_o' = I_o\left(1 - \frac{a_p(\lambda)}{a_p(\lambda)+s_p(\lambda)}\right) \quad . \tag{65}$$

For phytoplankton, absorption must be accounted for directly, since fluorescence will occur after the photon has been absorbed. When phytoplankton is contacted it is first decided if scattering or absorption is to be simulated by comparing the relative probability of these two events to a randomly selected number. If scattering is to be simulated we proceed as described in the previous paragraphs. If absorption is to be simulated, we assume that the photon will be absorbed and subsequently fluoresced at the fluorescent wavelength, λ_F. If the photon's wavelength is λ_F before absorption we assume that it will be lost upon any further absorption by phytoptankton.

Photon Path Length

The distance, d_j, that a photon travels between events is selected from a distribution function of the form

$$d_j = -\frac{1}{\alpha_T(\lambda)} \ln(\varepsilon) \tag{66}$$

Again ε is a random number on the range 0 to 1, and $\alpha_T(\lambda)$ is the total attenuation coefficient for a photon of wavelength λ.

Fluorescent Efficiency

Since all absorbed photons will not be fluoresced, in our simulations the weight of the photon is adjusted and fluorescence is forced to occur.

The fluorescent efficiency of the photon, η, is assumed to be related to the fluorescent cross section and the concentration of phytoplankton. (See Appendix 2).

$$\eta(\lambda) = \frac{\sigma(\lambda)CN_a m}{Ka(\lambda)W} \quad , \tag{67}$$

where

σ = fluorescent cross section (cm^2/molecule)

C = concentration of phytoplankton (cells/ml)

N_a = Avagadro's number

W = mass per mole of chlorophyll a

m = mass per cell

K = fraction of photons absorbed by phytoplankton that gets absorbed by chlorophyll a

$a(\lambda)$ = absorption coefficient of phytoplankton at wave-length λ.

For our analysis K is assumed to be unity. The adjusted weight of the photon after fluorescence is given by

$$I_o' = \eta I_o \quad . \tag{68}$$

Fluorescent Phase Function

When the photon is fluoresced the cosine of the polar angle of emission is assumed evenly distributed. The polar angle is then selected using the function

$$\cos\theta' = 2\varepsilon_1 - 1, \tag{69}$$

and the azimuthal angle is given by

$$\phi' = \pi(2\varepsilon_2 - 1) \quad . \tag{70}$$

Computer Model

Two computer programs, CARLO 1 and CARLO 4, were developed for the

Monte Carlo model. The first program is listed in Appendix 3. CARLO 1 is a single color group model and CARLO 4 is a four color group model. Both programs were written in BASIC-PLUS in EXTEND mode for execution on the PDP11/34 computer with RSTS/E operating system.

Lines 150-490 of the program include program input variables. A list of input variables and their functions follows the program listing in Table A1. Lines 700-995 initialize program parameters. Lines 1000-1010 begin the loop for each photon and lines 1100-1140 begin the loop for each event by calculating the distance the photon will travel (in line 1130) and testing its weight. The photon's position is calculated at line 1150 and lines 1170-1340 determine if any boundaries are contacted. Lines 1350-1420 correct the photon's location if boundaries are contacted. Lines 1460-1700 determine the appropriate action if boundaries were contacted. Lines 1720-1770 control program parameters and flow for cases in which boundaries are not contacted. Lines 1805-1880 calculate direction cosines. The events counter and photons counter are incremented in lines 3000 and 4000 and a summary is presented in lines 5000-5020. An analysis of the returned photons is done in lines 11000-11290. Lines 19200-19260 and 19500-19699 are for various outputs. Program functions are defined in lines 19290-19310.

Anacystis Marinus

An anacystis marinus culture, grown by NASA-Langley personnel (Poole) was used to provide optical data for the Monte Carlo model. This culture will be referred to as AM480.

The absorption measurements for AM480 were made with a spectra absorption coefficient instrument, SPACI, (Friedman, et al). Total attenuation coefficient measurements were taken with a small angle scattering meter, SASM. This instrument is similar in dësign and concept to the Scripps Institute of Oceanography ALSCAT (Austin and Petzold), except the SASM used cells of various length to allow for high turbidity measurement rather than in situ as employed by the ALSCAT. To obtain the volume scattering function, $\beta(\theta)$, small angle measurements, less than 25^{o}, were made with the SASM. Large angle measurement 25^{o} to 155^{o}, were made with a modified Brice Phoenix light scattering photometer. These modifications were made to achieve the same spectral range and resolution as the SASM. The complete volume scattering function was obtained by cubic spline fits to these data. The appropriate scattering probability distribution, $P(\theta)$, was determined by normalization and integration of the volume scattering function.

$$P(\theta) = \int_{\Omega} \frac{\beta(\theta)}{s} d\Omega \tag{71}$$

$$= \frac{2\pi}{s} \int_{0}^{\pi} \beta(\theta) \sin\theta d\theta \ . \tag{72}$$

The scattering coefficient s, was obtained by the subtracting the absorption coefficient from the total attenuation coefficient.

$$s = \alpha - a \ . \tag{73}$$

Figure 10 shows graphs of the scattering and absorption coefficients as a function of wavelength. The scattering probability distribution is shown in Figure 9. This distribution was assumed to be wavelength independent. For the simulations, incident photon wavelength of 454, 539, 598 and 617 nm were used. These values corresponded with those used in the NASA Airborne Lidar Oceanographic Probing Experiment, ALOPE, (Browell). The fluorescent wavelength used for the cholorphyll a molecule was 685 nm. A summary of the optical constants for AM480 is given in Table 1. To determine the fluorescent efficiencies several quantities that were not measured directly for AM480 were estimated from earlier data runs (Farmer).

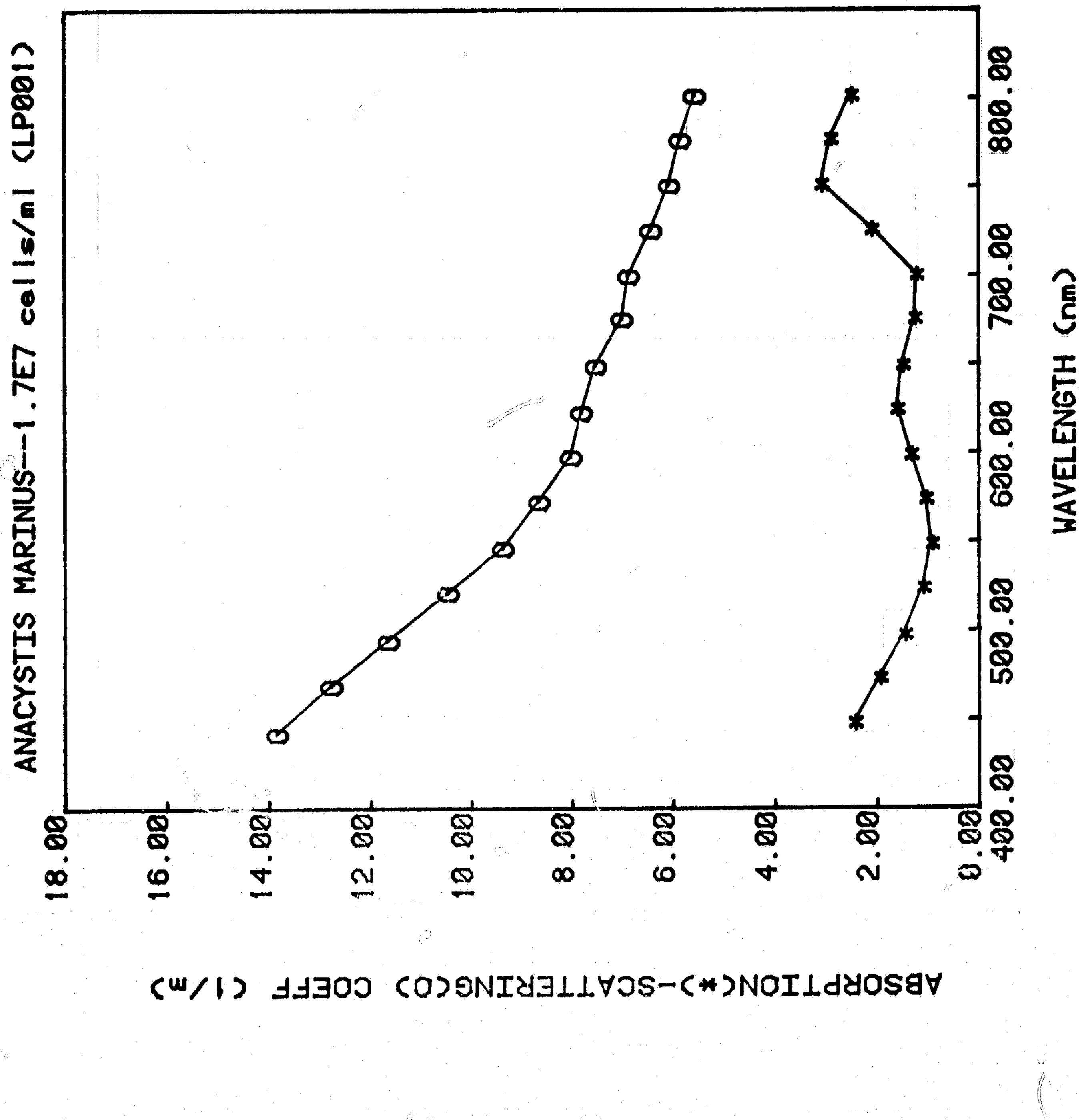
ANACYSTIS MARINUS--1.7E7 cells/ml (LP001)
ABSORPTION(*)-SCATTERING(O) COEFF (1/m)
WAVELENGTH (nm)
18.00
16.00
14.00
12.00
10.00
8.00
6.00
4.00
2.00
0.00
400.00
500.00
600.00
700.00
800.00

FIGURE 10

TABLE 1

OPTICAL PARAMETERS AM480

λ (nm)	a_{bulk} (m^{-1})	s_{bulk} (m^{-1})	a_{water} (m^{-1})	a_{chlo} (m^{-1})	σ_F (m^2/molecule)	η
454	2.3	13.7	.03	2.27	0.1×10^{-21}	.0025
539	0.9	9.8	.05	0.85	0.2×10^{-21}	.013
598	1.2	9.1	.19	1.01	1.0×10^{-21}	.049
617	1.4	7.8	.25	1.15	1.7×10^{-21}	.073
685	1.2	7.0	.45	.75	-	-

These included a cell concentration, 1.7 cell/ml, a mass per cell of 5.1 X 10^{-15} g/cell and the scattering cross sections σ_F, given in Table 1. The molecular weight of chlorophyll a was taken to be 893 g/mole. Since pure water attributed to the total measured absorption coefficient, absorption coefficient values for water (Smith and Taylor) were subtracted from the total measured values to give absorption coefficients for chlorophyll a.

Simulation Results

To provide input for the computer model, optical parameters were linearly extrapolatedover a concentration range of 1 X 10^6 cells/ml to 1 X 10^8 cells/ml. All photons that were backscattered within a radius of 1 meter of the origin were collected and analyzed. The normalized weights of the returned photons were plotted against $f(\alpha')$ where

$$f(\alpha') = \frac{C}{\alpha(\lambda)(1-\omega(\lambda)F) + \alpha(685)(1-\omega(685)F)} \tag{74}$$

and C is the concentration of chlorophyll a and F is the fraction of photons scattered in the forward direction. The quantity $\omega(\lambda)$ is the scattering albedo and is given by

$$\omega(\lambda) = \frac{s(\lambda)}{\alpha(\lambda)}. \tag{75}$$

A graph of $f(\alpha')$ versus concentration is given in Figure 11. A value of F = .98, obtained from the probability distribution given in Figure 9 was used in these plots.

Theoretical analysis (Browell) suggests that we might expect a linear dependence for the power received at a detector on $f(\alpha')$. Here we have introduced the quantity

$$\alpha'(\lambda) = \alpha(\lambda)(1-\omega(\lambda)F) \tag{76}$$

to partially account for the effects of multiple scattering.

Our preliminary results are presented in Figures 12-15 and summarized

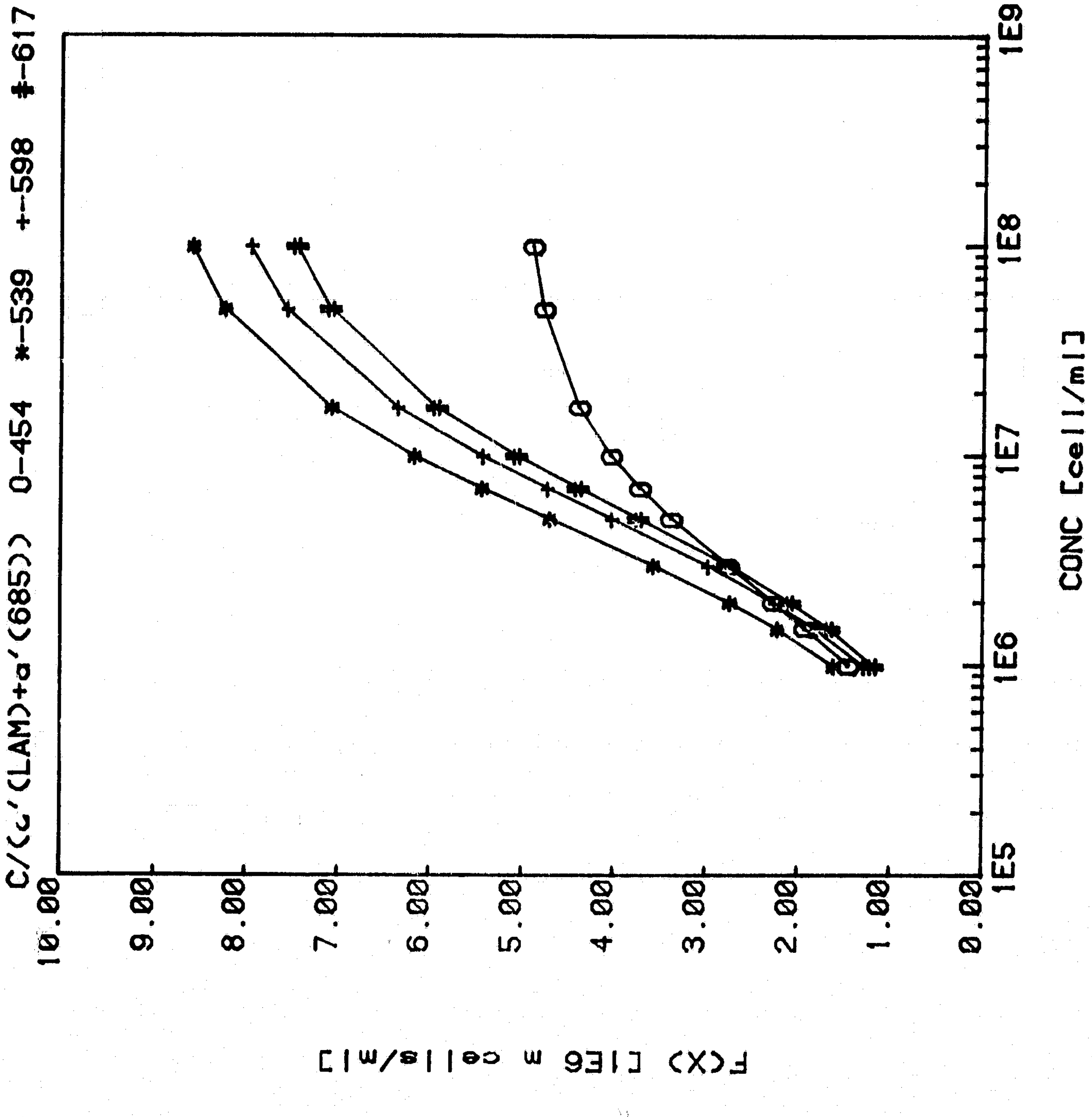
C/(c'(LAM)+a'(685)) 0-454 *-539 +-598 #-617
F(X) [1E6 m cells/ml]
10.00
9.00
8.00
7.00
6.00
5.00
4.00
3.00
2.00
1.00
0.00
1E5
1E6
1E7
1E8
1E9
CONC [cell/ml]

FIGURE 11

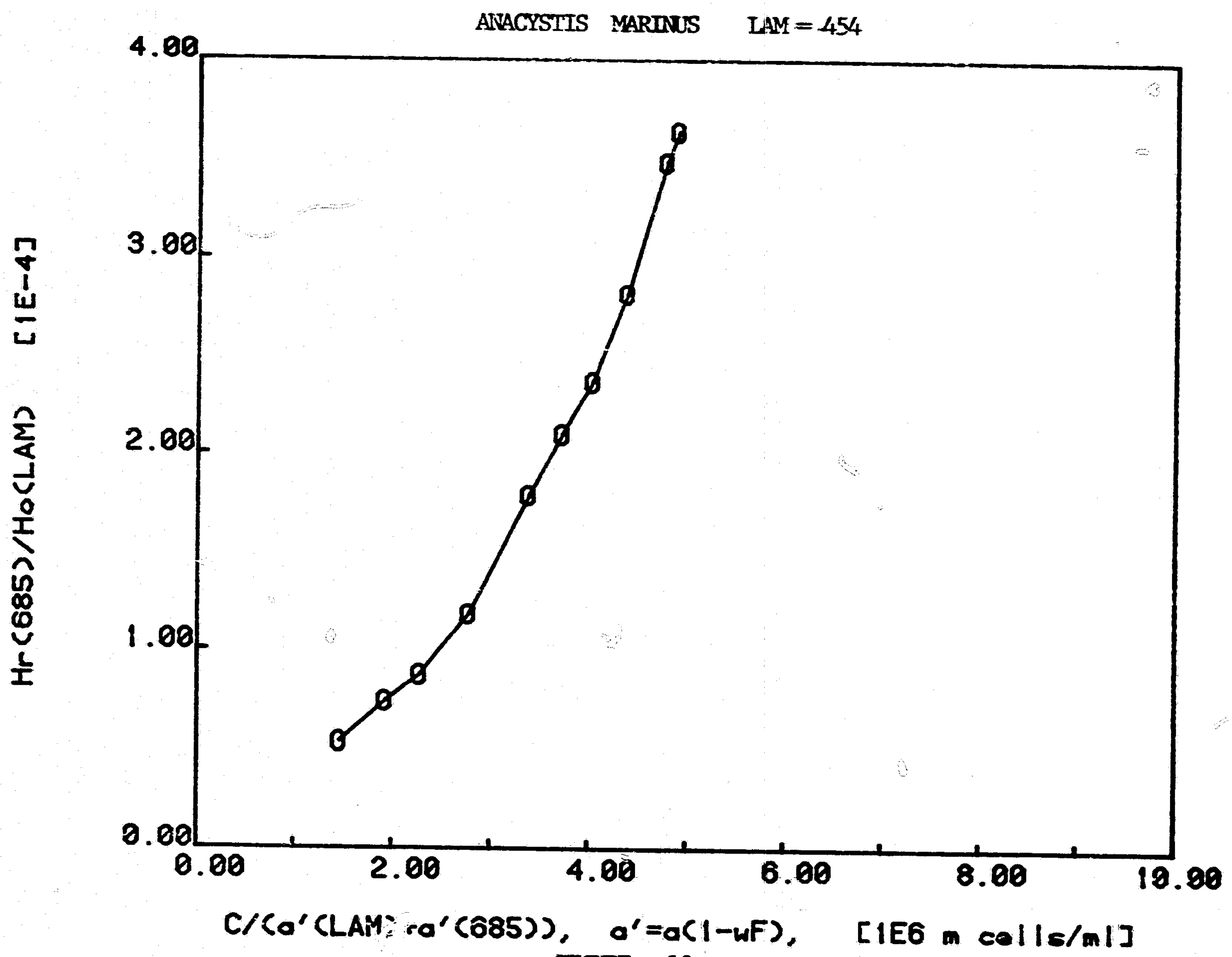
ANACYSTIS MARINUS LAM = 454
4.00
3.00
2.00
1.00
0.00
Hr(685)/Ho(LAM) [1E-4]
0.00
2.00
4.00
6.00
8.00
10.00
C/(a'(LAM)+a'(685)), a'=a(1-wF), [1E6 m cells/ml]

FIGURE 12

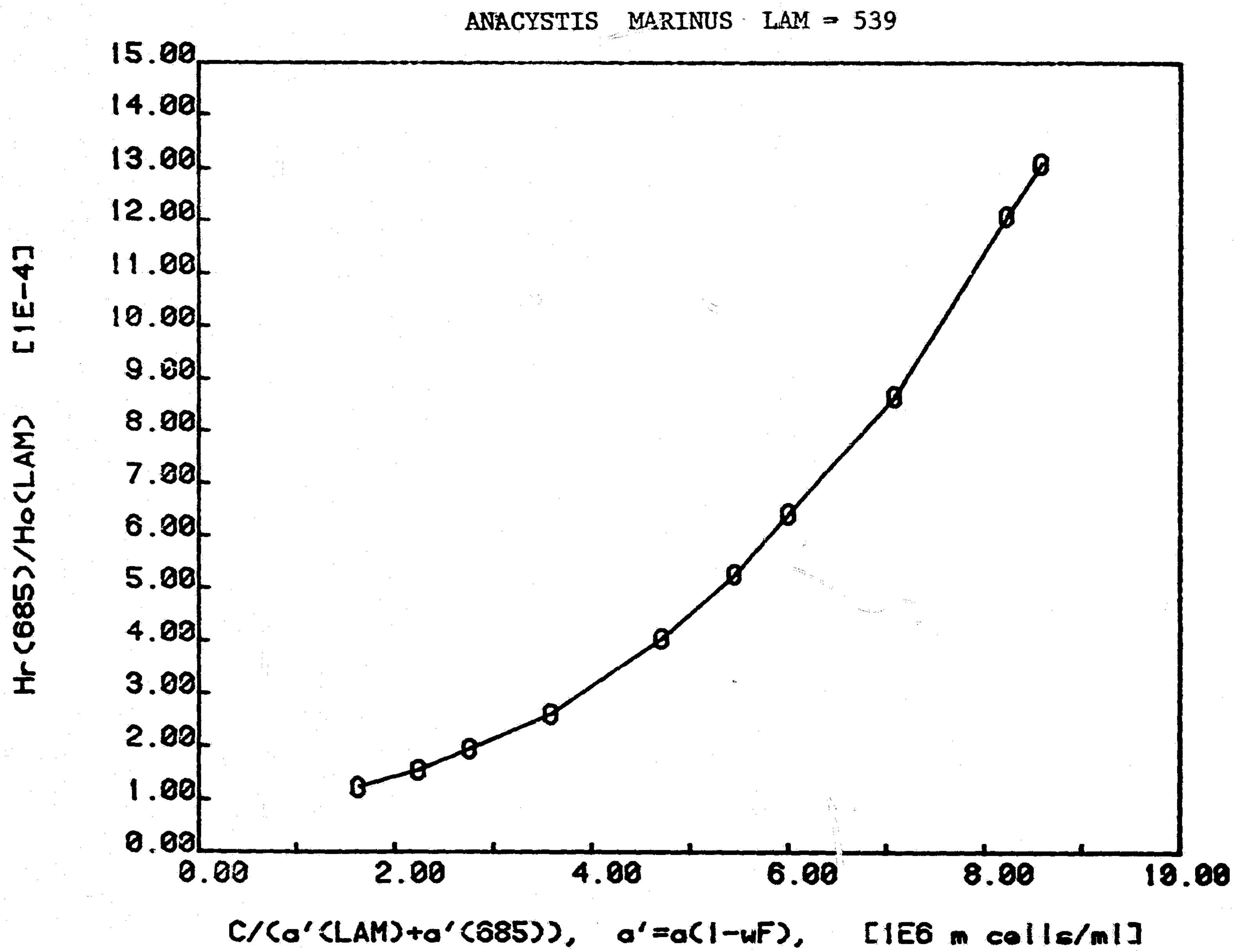
ANACYSTIS MARINUS LAM = 539
15.00
14.00
13.00
12.00
11.00
10.00
9.00
8.00
7.00
6.00
5.00
4.00
3.00
2.00
1.00
0.00
Hr(685)/Ho(LAM) [1E-4]
0.00
2.00
4.00
6.00
8.00
10.00
C/(a'(LAM)+a'(685)), a'=a(1-wF), [1E6 m cells/ml]

FIGURE 13

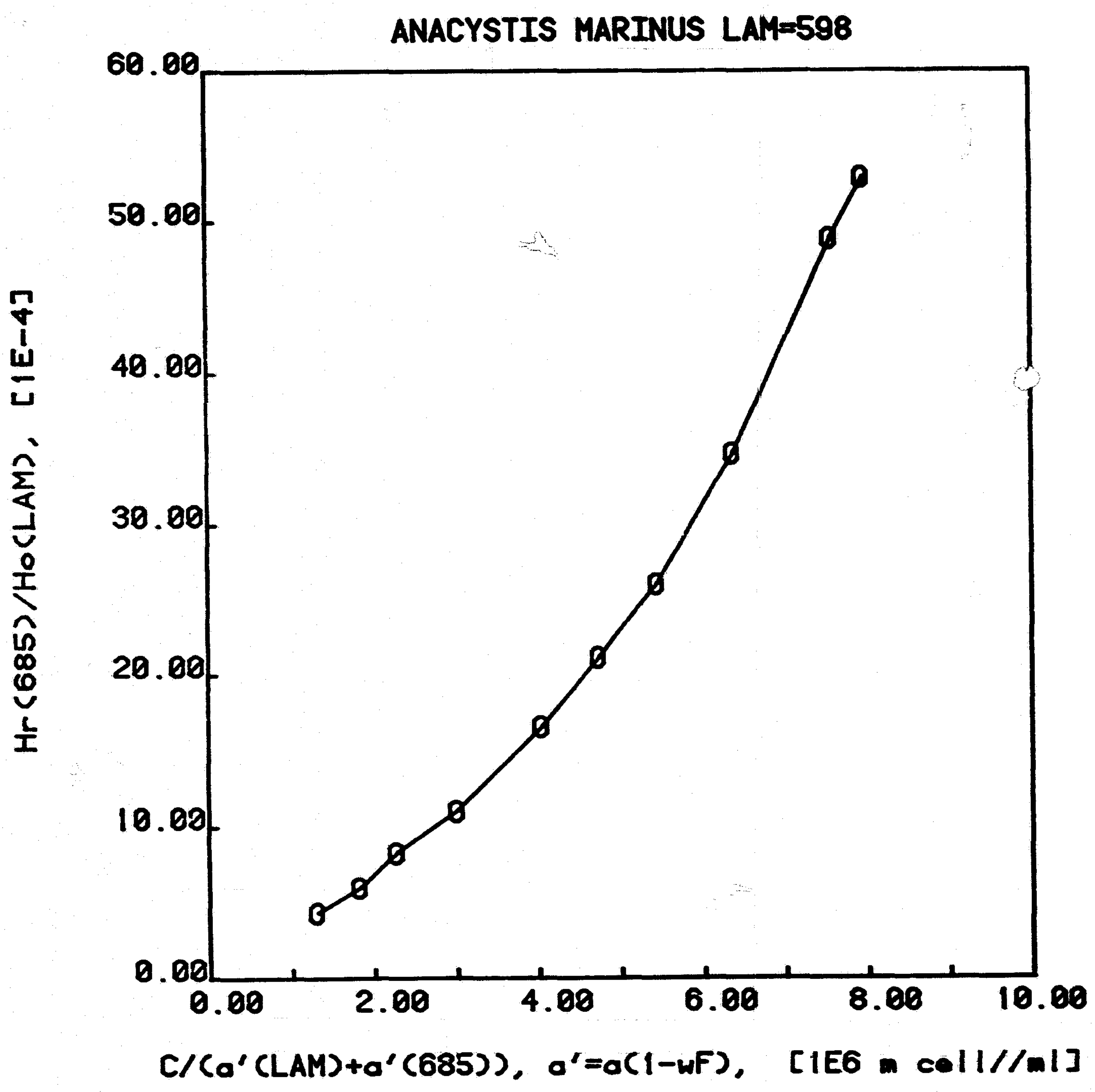
ANACYSTIS MARINUS LAM=598
60.00
50.00
40.00
30.00
20.00
10.00
0.00
0.00
2.00
4.00
6.00
8.00
10.00
Hr(685)/Ho(LAM), [1E-4]
C/(a'(LAM)+a'(685)), a'=a(1-wF), [1E6 m cell//ml]

FIGURE 14

ANACYSTIS MARINUS LAM = 617

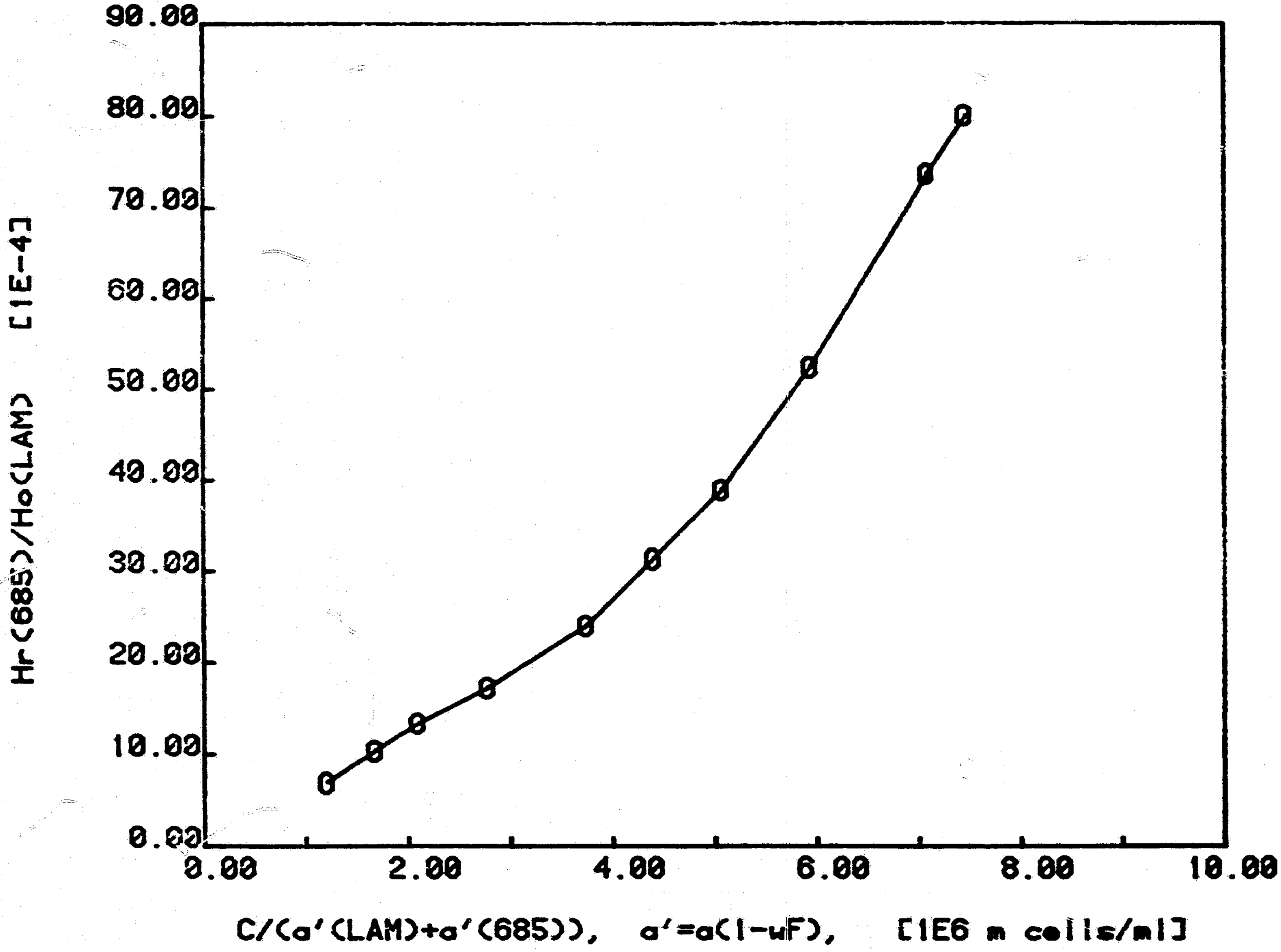

FIGURE 15

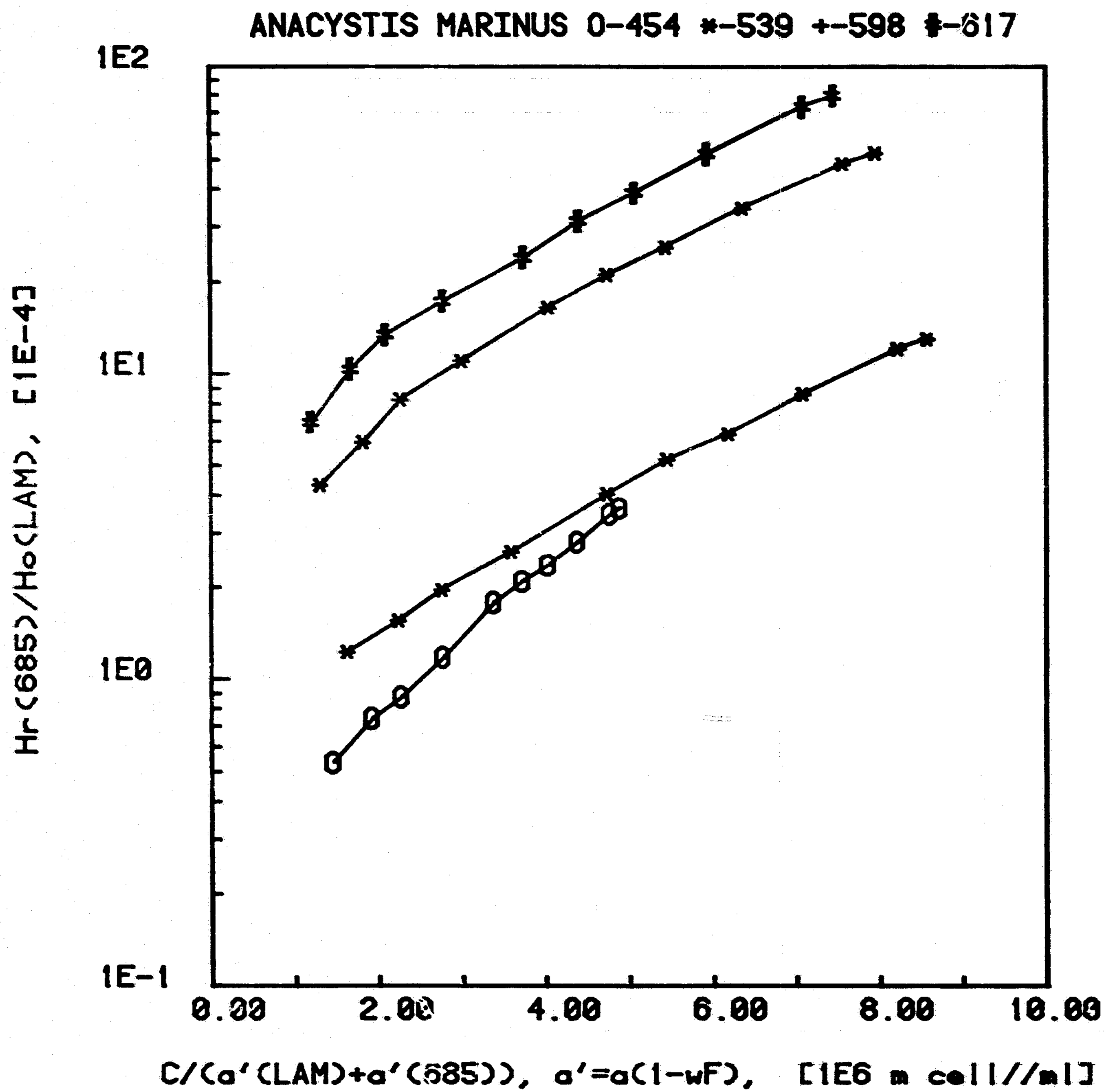
ANACYSTIS MARINUS O-454 *-539 +-598 #-617
1E2
1E1
1E0
1E-1
Hr(685)/Ho(LAM), [1E-4]
0.00
2.00
4.00
6.00
8.00
10.00
C/(a'(LAM)+a'(685)), a'=a(1-wF), [1E6 m cell//ml]

FIGURE 16

in Figure 16. The dependent axis in each of these plots is the accumulated weight of photons that are returned at the fluoresced wavelength, normalized by the accumulated weight (number of photons) incident at the exciting wavelength.

These analyses show a tendency for exponential behavior at high concentrations. However these results cannot be used as a conclusive test of the type of dependence on equation (74) because target geometry of the ALOPE system is not fully simulated. In addition, errors in the estimated sample properties can affect the results. To correct this latter problem, another culture is being grown for analysis. A complete measurement set will be made for this specimen.

Detector geometry can be fully simulated by special techniques. Consider the case of a finite detector a height z_o above the water surface. See Figure 17. Any event occurring within the interaction volume has a finite probability of contributing to the detector signal. When a photon undergoes a scattering event in the interaction volume the probability that the photon will be detected is given by ΔP_A where

$$\Delta P_A = \int_{\Omega_A} \frac{\beta(\theta)}{s} d\Omega_A \quad , \tag{77}$$

and Ω_A is the solid angle subtended by the detector aperture relative to the current photon position. This integral can be approximated by

$$\Delta P_A = \frac{\beta(\theta')}{s} \Omega_A \quad , \tag{78}$$

where θ' is the scattering angle that will cause the photon to travel in a direction toward the center of the detector aperture.

At each scattering event the contribution to the detector signal, W, is calculated where

$$W = I_{oj} e^{-\alpha d} \quad \Delta P_A \left(\frac{s}{a+s}\right) \tag{79}$$

In equation (79), I_{oj} is the weight of the photon prior to undergoing the jth scattering event and the quantity

$$\frac{s}{a+s}$$

is the probability that the photon will be scattered (as opposed to being absorbed). The path length from the photon to the top of the water surface is d and the total attenuation of the medium is α. Then the quantity $e^{-\alpha d}$ represent the survival probability of the photon while traveling toward the detector.

Photons can be forced to remain within the interaction volume by selecting the distance that the photon travels between events, d_j, from a truncated distribution function and correspondingly adjusting the photon's weight. If the path length from the photon to the edge of interaction volume is d_E, then d_j is given by (Kattawa)

$$d_j = -\ln(1-\varepsilon(1-e^{-\alpha d_E}))/\alpha \tag{80}$$

and the corresponding weight adjustment is given by

$$I_{oj} = I_o(1-e^{-\alpha d_E}) \tag{81}$$

and

$$d_E = d_w + \sin\delta \frac{d_w \cos\theta + z}{\sin\,(\theta-\delta)} \quad , \delta < \theta. \tag{82}$$

We are presently implementing these procedures in our Monte Carlo computer model.

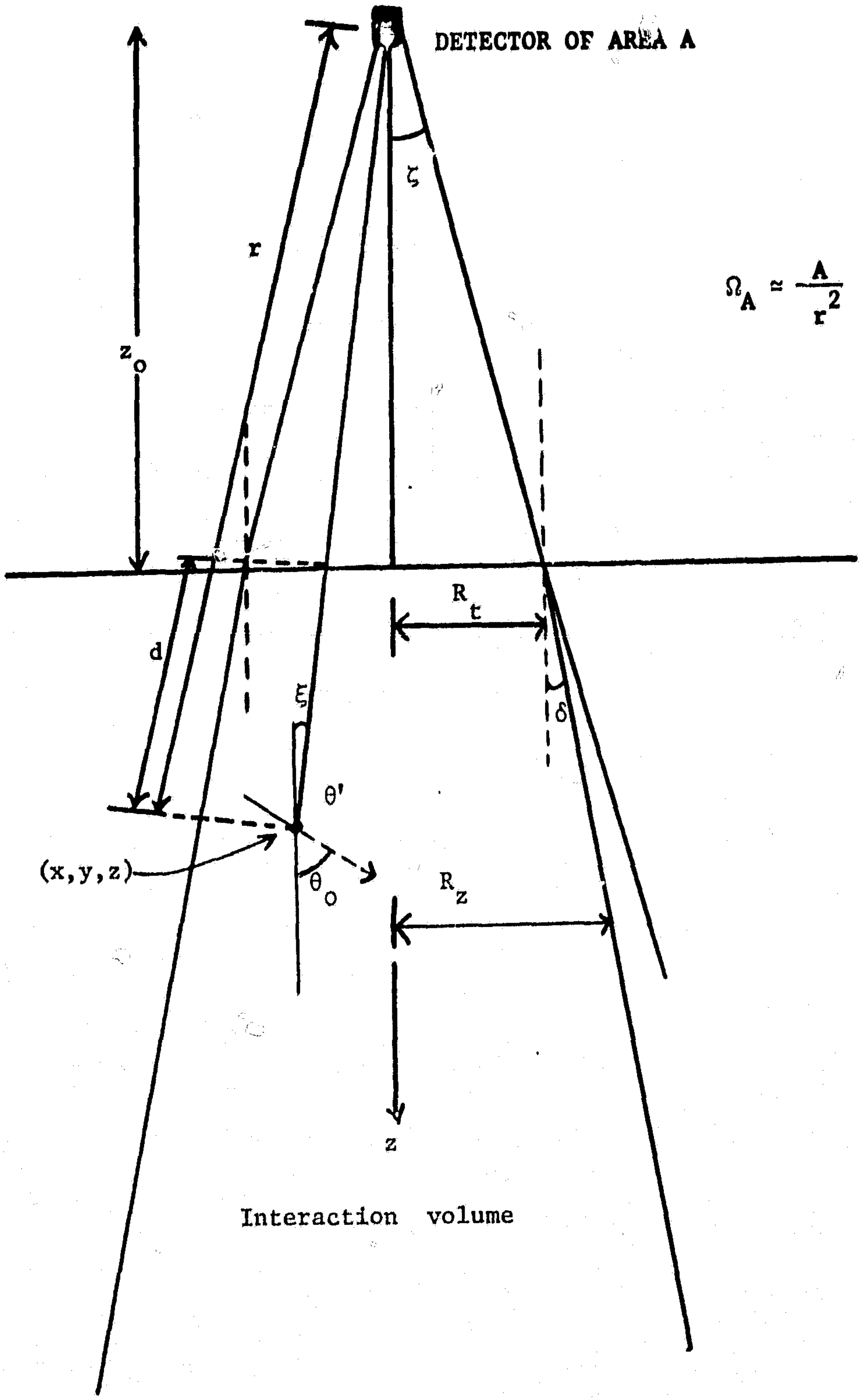
DETECTOR OF AREA A
ζ
r
$\Omega_A \approx \frac{A}{r^2}$
z_o
R_t
d
ξ
δ
θ'
(x,y,z)
θ_o
R_z
z
Interaction volume

FIGURE 17

Appendix 1

WEIGHINC TECHNIQUE (Poole)

The number of events occurring in a distance x is distributed as a Poisson distribution written in a spatial rather than temporal sense, or

$$P_m(x) = \frac{(\alpha x)^m}{m!} e^{-\alpha x} \tag{1-1}$$

where x = distance traveled

m = number of events

α = attenuation coefficient.

As an alternative weighting technique for suspended particulates we multiply the photon's weight by the probability (P) of scattering for that event, where

$$P = \frac{s}{\alpha} = \tilde{\omega}_o \tag{1-2}$$

After a large number of photons have traveled a distance D, the expected value of the average photon weight, E(W), is

$$\begin{aligned} E(W) &= E\left[(\tilde{\omega}_o)^m\right] \\ &= \sum_{m=o}^{\infty} P_m(D)(\tilde{\omega}_o)^m \\ &= P_o(D)(1)+P_1(D)\tilde{\omega}_o+P_2(D)\tilde{\omega}_o^{\,2}+ \ldots \end{aligned} \tag{1-3}$$

Substitution from equation (1-1) for $P_m(x)$ yields

$$\begin{aligned} E\ (\tilde{\omega}_o)^m &= e^{-\alpha D} + \frac{\alpha D}{1!} e^{-\alpha D}\, \tilde{\omega}_o + \frac{(\alpha D)^2}{2!} e^{-\alpha D}\, \tilde{\omega}_o^{\,2} + \ldots \\ &= e^{-\alpha D}\left[1 + \frac{\alpha D}{1!}\tilde{\omega}_o + \frac{(\alpha D\, \tilde{\omega}_o)^2}{2!} + \ldots\right] \\ &= e^{-\alpha D}\, e^{\alpha D \tilde{\omega}_0} \\ &= e^{-\alpha D}\, e^{sD} = e^{-(\alpha-s)D} = e^{-aD}\ . \end{aligned} \tag{1-4}$$

Appendix 2

FLUORESCENT EFFICIENCY CALCULATION

Consider the fluorescent efficiency, η, where

$$\eta = \frac{\text{\# of photons fluoresced by cholorophyll } \underline{a}}{\text{\# of photons absorbed by cholorophyll } \underline{a}}$$

$$= \frac{I_F}{I_o K \frac{a}{\alpha}} \qquad (2\text{-}1)$$

and a = absorption coefficient for medium

α = attenution coefficient for medium

$\frac{a}{\alpha}$ = probability of absorption by the medium

K = fraction of absorption photons that are absorbed by cholorophyll a

The fluorescent cross section, σ, is

$$\sigma = \frac{\text{\# of photon fluoresced}}{\text{\# of photon incident x \# of molecules per cm}^2} = \frac{I_F}{I_o N} .$$

Therefore,
$$\eta = \frac{\sigma N}{K\frac{a}{\alpha}} . \qquad (2\text{-}2)$$

Also C = concentration in cell/cm^3

N_A = number of molecules per mole

W = number of grams per mole

m = number of grams per cell

ℓ = mean free path length of photon = $\frac{1}{\alpha}$

$$C \left(\frac{\text{cell}}{\text{cm}^3}\right) = N \left(\frac{\text{molecules}}{\text{cm}^2}\right) \frac{1}{N_A \left(\frac{\text{molecules}}{\text{mole}}\right)} W \left(\frac{\text{g}}{\text{mole}}\right) \frac{1}{m\left(\frac{\text{g}}{\text{cell}}\right)} \frac{1}{\ell(\text{cm})}$$

$$N \left(\frac{\text{molecules}}{\text{cm}^2}\right) = \frac{C \left(\frac{\text{cell}}{\text{cm}^3}\right) N_A \left(\frac{\text{molecules}}{\text{mole}}\right) m \left(\frac{\text{g}}{\text{cell}}\right) \ell \text{ (cm)}}{W \left(\frac{\text{g}}{\text{mole}}\right)}$$

Then the quantum efficiency is given by

$$\eta = \frac{\sigma}{K\frac{a}{\alpha}} \frac{CN_A m\ \ell}{W} \tag{2-3}$$

or

$$\eta = \frac{\sigma C N_A m}{KaW} \quad . \tag{2-4}$$

If a normalized value for a is used then, η can be written as

$$\eta = \frac{\sigma N_A m}{Ka^* W}, \tag{2-5}$$

where $a^* = \frac{a}{C}$.

Appendix 3

PROGRAM LISTING

```
1!!!!!!!MONTECARLO           FLUORESCENCE MODEL!!!!!!!
2!!!!!!!-----CARLO1-----FEB 25 1980-------!!!!!!!
5!!!!!!!SECOND TEST CASE FOR CHLOROPHYLL MODEL
        HOMOGENEOUS CHLO
        NO PART.
        ANACYSTIS MARINUS-LP01
        INFINITE BOUNDS
        INPUT DATA L.POOLE


6!!!!!!!SINGLE COLOR GROUP MODEL!!!!!!!


10 EXTEND
40 DIM Q(3),DELQ(3),Q1(3),REFX(10,5),LDPTH(10,5),SCW(10,5),SCP(10,5),SCC(10,5),ACP(10,5),ACC(10,5),ACW(10,5),TAP(10,5)
42 DIM TAC(10,5),TAT(10,5),CPP(10,5),CPC(10,5),IMIN(5),TANK(5,5),W(3),W1(3),W4(3),ETA(5),Y(101)
150 !
    !
    !INPUT PARAMETERS
    !
    !
160 L0=2
170 LAM0=1
180 NPH=100
190 NEV=100
200 THET0=0
210 PHI0=0
219 FILE$='00'
220 FILE$='DM1:AM00'+FILE$+'.DAT'
225 TITLE$='ANACYSTIS MARINUS-4/80-1 COLOR MODEL'
230 R0=1
240 SCV$='SVLP01.DAT'
250 OUT$='KB:'
252 CONP=0
255 CONC=1.7E7
257 CONW=1
260 MINW=1E-3
270 ROUT=1
271 ROUT2=ROUT^2
279 TITLE$=TITLE$+' LAMDA='+NUM$(LAM0)+'CONC='+NUM$(CONC)+DATE$(0)
280 !
    !
    !DATA ARRAYS
    !
    !
300 MAT READ LDPTH(L0,5)!
310 DATA     0,      0,      0,      0,      0,
```

```
          0,     0,     0,     0,     0
320 MAT READ TANK!
330 DATA    0,     0,     0,     0,     0,
            0,     0,     0,     0,     0,
            0,     0,     0,     0,     0,
            0,     0,     0,     0,     0,
            0,     0,     0,     0,     0
340 MAT READ REFX(LO,5)!
350 DATA    1,     1,     1,     1,     1,
        1.33,  1.33,  1.33,  1.33,  1.33
360 MAT READ SCC(LO,5)
370 DATA  0,     0,     0,     0,     0,
      8.06E-7,5.74E-7,4.76E-7,4.59E-7,4.12E-7
380 MAT READ SCP(LO,5)
390 DATA      0,      0,      0,      0,      0,
              0,      0,      0,      0,      0
400 MAT READ ACC(LO,5)!
410 DATA      0,     0,     0,     0,     0,
        1.34E-7,.500E-7,.594E-7,.676E-7,.441E-7
420 MAT READ ACP(LO,5)!
430 DATA    0,     0,     0,     0,     0,
            0,     0,     0,     0,     0
440 MAT READ ACW(LO,5)!
450 DATA     0,     0,     0,     0,     0,
          .03,    .05,   .19,   .25,   .45
460 MAT READ ETA(5)!
470 DATA .00254,  .013, .0488, .0731,    0
480 MAT READ SCW(LO,5)!
490 DATA    0,     0,     0,     0,     0,
            0,     0,     0,     0,     0
700 !
    !
    !INITIALIZE PARAMETERS
    !
    !
705 MAT SCC=(CONC)*SCC
        \MAT ACC=(CONC)*ACC
        \MAT SCP=(CONP)*SCP
        \MAT ACP=(CONP)*ACP
        \MAT ACW=(CONW)*ACW
        \MAT SCW=(CONW)*SCW
710 MAT TAW=ZER(LO,5)
        \MAT TAP=ZER(LO,5)
        \MAT TAC=ZER(LO,5)
        \MAT TAT=ZER(LO,5)
720 OPEN SCV$ FOR INPUT AS FILE #2
        \OPEN OUT$ FOR OUTPUT AS FILE #4
820 MAT TAW=ACW+SCW
```

```
        \MAT TAP=ACP+SCP
        \MAT TAC=ACC+SCC
        \MAT TAT=TAP+TAC
830 FOR I=2 TO LO
        \FOR J=1 TO 5
        \CPP(I,J)=TAP(I,J)/TAT(I,J)
        \CPC(I,J)=TAC(I,J)/TAT(I,J)
        \NEXT J
        \NEXT I
840 FOR I=1 TO 5
        \TANK(5,I)=TANK(1,I)^2
        \LDPTH(LO,I)=TANK(2,I)
        \LDPTH(1,I)=0
        \NEXT I
850 ONE=1.00001
        \MAT IMIN=CON
        \INPUT #2,SCVT$
        \FOR I=1 TO 101
        \INPUT #2,Y(I)
        \NEXT I
        \IF Y(101)<>180.00 THEN STOP
852 MAT Y=(.017453)*Y
860 NPR=0
        \C$=','
        \IF NPH<=1000 THEN PO=1 ELSE PO=.02*NPH
870 MAT IMIN=(MINW)*IMIN
        \THETO=THETO*.017453
        \PHIO=PHIO*.017453
        \PHI=PHIO
        \THET=FNASN(SIN(THETO)/REFX(2,LAMO)*REFX(1,LAMO))
880 W3=SIN(THET)
        \W4(1)=W3*COS(PHI)
        \W4(2)=W3*SIN(PHI)
        \W4(3)=SQR(ONE-W3^2)
        \WR=FNR(REFX(1,LAMO)/REFX(2,LAMO),W4(3),W3,0)
890 FOR I=1 TO RO
        \D1=RND
        \NEXT I
        \OPEN FILE$ FOR OUTPUT AS FILE #1
        \GOSUB 19200
995 PRINT#1,TITLE$
        \CLOSE #2
1000 !
     !
     !START I-TH PHOTON
     !
     !
1010 FOR I=1 TO NPH
```

```
      \LL=2
      \LAM=LAM0
      \I0=1
      \MAT Q=ZER
      \MAT W=W4
      \W2=W3
      \EVC=0
      \THET1=0
      \PHI1=0
      \RATIO=1
      \IF RND<WR THEN 1670
1100 !
     !
     !START J-TH EVENT
     !
     !
1110 FOR J=1 TO NEV
1130 DJ=-LOG(RND)/TAT(LL,LAM)
      \EVC=EVC+1
1140 IF I0<IMIN(LAM) THEN J=NEV
      \GOTO 3000
1147 !
     !
     !SET TRIAL COORDINATE
     !
     !
1150 MAT DELQ=(DJ)*W
      \MAT Q1=Q+DELQ
1152 !
     !
     !DIAGNOSTIC OUTPUT
     !
     !
1154 GOTO 1160
1155 GOSUB 19600
1160 !
     !
     !DETERMINE IF BOUND, CONTACTED
     !
     !
1170 BR=0
      \CG=0
      \RATIO=1
      \DJBND=-1
      \IF(Q1(1)^2+Q1(2)^2)<TANK(5,LAM) OR TANK(5,LAM)=0 THEN WCP=0 ELSE WCP=-1
1180 IF W(3)<0 THEN PMD=-1
      \GOTO 1250
1190 PMD=1
```

```
      \IF Q1(3)<LDPTH(LL+0,LAM) OR LDPTH(LL+0,LAM)=0 THEN 1310
1200 DJTOB=(LDPTH(LL+0,LAM)-Q(3))/W(3)
      \IF WCP=0 THEN 1230
1210 SXW=(Q(1)*W(1)+Q(2)*W(2))/W2
      \DJWALL=-SXW+SQR(SXW^2+TANK(5,LAM)-(Q(1)^2+Q(2)^2))
      \DJWALL=DJWALL/W2
1220 IF DJWALL<DJTOB THEN 1330
1230 IF LDPTH(LL+0,LAM)=TANK(2,LAM) THEN BR=3 ELSE BR=2
1240 DJBND=DJTOB
      \GOTO 1340
1250 IF Q1(3)>LDPTH(LL-1,LAM) THEN 1310
1260 DJTOB=(LDPTH(LL-1,LAM)-Q(3))/W(3)
      \IF WCP=0 THEN 1290
1270 SXW=(Q(1)*W(1)+Q(2)*W(2))/W2
      \DJWALL=-SXW+SQR(SXW^2+TANK(5,LAM)-(Q(1)^2+Q(2)^2))
      \DJWALL=DJWALL/W2
1280 IF DJWALL<DJTOB THEN 1330
1290 IF LDPTH(LL-1,LAM)=0 THEN BR=4 ELSE BR=5
1300 DJBND=DJTOB
      \GOTO 1340
1310 IF WCP=0 THEN 1350
1320 SXW=(Q(1)*W(1)+Q(2)*W(2))/W2
      \DJWALL=-SXW+SQR(SXW^2+TANK(5,LAM)-(Q(1)^2+Q(2)^2))
      \DJWALL=DJWALL/W2
1330 DJBND=DJWALL
      \BR=1
1340 RATIO=DJBND/DJ
1350 !
     !
     !UPDATE IO,X,Y,Z, AND BRANCH TO TYPE OF CONTACT
     !
     !
1410 IO=IO*EXP(-ACU(LL,LAM)*RATIO*DJ)
1415 IF BR=0 THEN MAT Q=Q1
      \GOTO 1460
1420 MAT DELQ=(RATIO)*DELQ
      \MAT Q=Q+DELQ
1460 ON 1+BR GOTO 1720,1500,1540,1610,1640,1540
1500 !
     !
     !WALL CONTACTED
     !
     !
1510 PHI1=PI*(2*RND-1)
      \D1=RND
      \A=SQR(ONE-D1)
      \B=SQR(D1)
      \W(1)=-Q(1)/TANK(1,LAM)
```

```
      \W(2)=-Q(2)/TANK(1,LAM)
      \W(3)=0
      \B1=B*COS(PHI1)
1520 B2=B*SIN(PHI1)
      \W1(1)=-B2*W(2)+A*W(1)
      \W1(2)=B2*W(1)+A*W(2)
      \W1(3)=-B1
      \W2=SQR(ONE-B1^2)
      \MAT W=W1
1530 I0=I0*TANK(3,LAM)
      \GOTO 3000
1540 !
     !
     !LAYER BOUND CONTACTED
     !
     !
1560 IF REFX(LL,LAM)=REFX(LL+PMD,LAM)THEN 1603
1570 IF REFX(LL,LAM)*W2/REFX(LL+PMD,LAM)>1 THEN W(3)=-W(3)
      \GOTO 1605
1580 IF RND<FNR(REFX(LL,LAM)/REFX(LL+PMD,LAM),W(3),W2,0) THEN W(3)=-W(3)
      \GOTO 1605
1590 D1=REFX(LL,LAM)/REFX(LL+PMD,LAM)
      \W(1)=D1*W(1)
      \W(2)=D1*W(2)
      \W2=D1*W2
      \W(3)=SGN(W(3))*SQR(ONE-W2^2)
1603 DJ=DJ*TAT(LL,LAM)/TAT(LL+PMD,LAM)
      \LL=LL+PMD
1605 DJ=(1-RATIO)*DJ
      \IF DJ>1E-5 THEN 1140 ELSE 3000
1610 !
     !
     !BOTTOM CONTACTED
     !
     !
1620 PHI1=PI*(2*RND-1)
      \D1=RND
      \W(3)=-SQR(ONE-D1)
      \B=SQR(D1)
      \W(1)=-B*COS(PHI1)
      \W(2)=B*SIN(PHI1)
      \W2=B
1630 I0=I0*TANK(4,LAM)
      \GOTO 3000
1640 !
     !
     !SURFACE CONTACTED
     !
```

```
     !
1650 IF REFX(2,LAM)*W2>1 THEN W(3)=-W(3)
       \DJ=(1-RATIO)*DJ
       \IF DJ>1E-5 THEN 1140 ELSE 3000
1660 D1=FNR(REFX(2,LAM)/REFX(1,LAM),W(3),W2,0)
       \I0=I0*(1-D1)
1670 THET2=FNASN(REFX(2,LAM)*W2)
       \PHI2=ATN(W(2)/W(1))
1680 J=NEV
       \NPR=NPR+1
       \IF NPR/PO=INT(NPR/PO) THEN GOSUB 19500
1690 PRINT#1,Q(1);C$;Q(2);C$;I0;C$;THET2;C$;PHI2;C$;LAM;C$;EVC;C$;I
1700 GOTO 3000
1720 !
     !
     !PARTICLE CONTACTED, DETERMINE TYPE
     !
     !
1730 IF RND>CPC(LL,LAM) THEN 1780
1740 IF RND>ACC(LL,LAM)/TAC(LL,LAM) THEN 1760
1746 !
     !
     !CHLO ABS OR FLUO
     !
     !
1750 I0=I0*ETA(LAM)
       \LAM=5
       \PHI1=PI*(2*RND-1)
       \W(3)=2*RND-1
       \W2=SQR(ONE-W(3)^2)
       \W(1)=W2*COS(PHI1)
       \W(2)=W2*SIN(PHI1)
       \GOTO 3000
1760 !
     !
     !CHLO SCATTERING
     !
     !
1770 GOTO 1810
1780 !
     !
     !PART CONTACT ADJ FOR ABS AND FORCE SCATTERING
     !
     !
1790 I0=I0*(1-ACP(LL,LAM)/TAP(LL,LAM))
1800 GOTO 1810
1805 !
     !
```

```
     !DIRECTION COSINES
     !
     !
1810 D1=100*RND
        \D2=1+INT(D1)
        \THET1=Y(D2)+(Y(D2+1)-Y(D2))*(D2-D1)
1820 PHI1=PI*(2*RND-1)
1830 A=COS(THET1)
        \B=SIN(THET1)
1840 B1=B*COS(PHI1)
        \B2=B*SIN(PHI1)
        \IF ABS(W(3))>.999 THEN 1870
1850 W1(1)=(W(1)*W(3)*B1-W(2)*B2)/W2+A*W(1)
        \W1(2)=(W(2)*W(3)*B1+W(1)*B2)/W2+A*W(2)
        \W1(3)=-W2*B1+W(3)*A
1860 GOTO 1880
1870 W1(1)=B1*W(3)
        \W1(2)=B2
        \W1(3)=A*W(3)
1880 MAT W=W1
        \IF W(3)<=1 THEN W2=SQR(1-W(3)^2) ELSE W2=0
1900 !
     !
     !
     !
     !
3000 NEXT J
4000 NEXT I
5000 PRINT#4,NPH;' PHOTONS RUN ';NPR;' PHOTONS RETURNED '
5010 PRINT#4,'TOTAL TIME(SEC) = ';TIME(0)-TIM0;'CPU TIME(SEC) = ';(TIME(1)-TIM1)/10;'KCT'S = ';TIME(3)-TIM3
5020 CLOSE #1
5090 !
     !
     !
     !
     !
11000  !!!!!!MCWGHT----- WEIGHT ANALYSIS FOR MONTECARLO DATA---!!!!!
11001 !
      !
      !
11015 OPEN FILE$ FOR INPUT AS FILE #3%
11040 PRINT#4%,
        \PRINT#4%,'WEIGHT ANALYSIS FOR FILE: ';FILE$
        \PRINT#4%,
11050 INPUT#3%,T$
        \PRINT#4%,T$
        \PRINT#4%,
        \DIM W9(9%)
```

```
       \MAT W=ZER
       \ON ERROR GOTO 11200
11100 INPUT #3,X,Y,W0,T,P,F,J,I
11105

      IF X^2+Y^2>ROUT2 THEN 11100   !!!   RESTRICT OUTPUT RAD TO ROUT METER



11110 !!!!!!DIAGNOSTIS PRINT#4%, OUT!!!!!!
11120 GOTO 11140
11130 PRINT#4%, USING' ####.## ####.## #.###### ###.## ###.## # ### #####', X,Y,W0,T,P,F,J,I
11140 W9(1)=W9(1)+W0
       \W9(6)=W9(6)+W0*COS(T)
       \W9(5)=W9(5)+1
       \IF J=0 THEN W9(2)=W9(2)+W0
       \W9(7)=W9(7)+W0*COS(T)
       \GOTO 11100
11150 IF F=5 THEN W9(3)=W9(3)+W0
       \W9(8)=W9(8)+W0*COS(T)
       \GOTO 11100
11160 W9(4)=W9(4)+W0
       \W9(9)=W9(9)+W0*COS(T)
       \GOTO 11100
11200 IF ERR<>11 THEN ON ERROR GOTO 0
11210 PRINT#4%, 'END OF FILE'
11220 PRINT #4%,
       \PRINT #4%,'MAX RADIUS OUT: ';ROUT;' M'
       \PRINT #4%,
11230 PRINT#4%, 'WEIGHTS: TOTAL WEIGHT-----';W9(1),' COS ADJ ';W9(6)
11240 PRINT#4%, '         SPECULAR REFL----';W9(2),'         ';W9(7)
11250 PRINT#4%, '         WGHT(685)--------';W9(3),'         ';W9(8)
11260 PRINT#4%, '         WGHT(LAMDA)------';W9(4),'         ';W9(9)
11270 PRINT#4%, '         # PHOTONS RET----';W9(5)
11280 CLOSE #3%
       \CLOSE #4%
11290 GOTO 32373
19090 STOP
19200 !
      !PARAMETERS PRINT#4,OUT
      !
19205 PRINT#4,
       \PRINT#4,'FILE NAME: ';FILE$
       \PRINT#4,
19207 PRINT #4%,'SCATTERING VECTOR: ';SCVT$
       \PRINT #4%,'CONC CHLO: ';CONC
       \PRINT #4%,'CONC PART: ';CONP
       \PRINT #4%,'CONC WATER: ';CONW
```

```
      \PRINT #4%,'LANDA PARAM: ';LAMO
      \PRINT #4%,'STEP#1: ';LO
      \PRINT #4%,'WGHT MIN: ';MINW
19210 PRINT#4,'LAYER DEPTH'
      \MAT PRINT#4,LDPTH,
      \PRINT#4,'REFRACTIVE INDEX'
      \MAT PRINT#4,REFX,
      \PRINT#4,'SCAT COEF PART,'
      \MAT PRINT#4,SCP,
19220 PRINT#4,'SCAT COEF CHLO,'
      \MAT PRINT#4,SCC,
      \PRINT#4,'ABS COEF PART,'
      \MAT PRINT#4,ACP,
      \PRINT#4,'ABS COEF CHLO,'
      \MAT PRINT#4,ACC,
19230 PRINT#4,'ABS COEF WATER'
      \MAT PRINT#4,ACW,
      \PRINT#4,'ETA'
      \MAT PRINT#4,ETA,
      \PRINT#4,'TANK PARAMETERS'
      \MAT PRINT#4,TANK,
19245 SLEEP 10
      \TIM0=TIME(0)
      \TIM1=TIME(1)
      \TIM3=TIME(3)
19250 PRINT#4,STRING$(4,10)
      \PRINT#4,'    X       Y     I0       THETA    PHI   LAM EVN PHOTON'
19260 RETURN
19290 !
     !DEF FN  ARCCOS   ARCSIN   FRESNEL REFL
     !
19300 DEF FNASN(X)=ATN(X/SQR(ONE-X^2))
      \DEF FNACS(X)=ATN(SQR(ONE-X^2)/X)-PI*(X<0)
19310 DEF FNR(A,B,C,D)
      \B=ABS(B)
      \D=SQR(1-(A*C)^2)
      \D1=D*B
      \D2=A*B
      \D3=A*C^2
      \FNR=.5*(((D2-D)/(D2+D))^2)*(1+((D1-D3)/(D1+D3))^2)
      \FNEND
19500 !
     !TERMINAL PRINOUT
     !
19510 PRINT#4,USING '####.## ####.## #.######   ###.## ###.##  #  ### #####',R(1),R(2),I0,THET2*57.296,PHI2*57.296,LAM,
EVC,I
19520 RETURN
19600 !
     !TERMINAL OUTPUT FOR DIAGNOSTICS
```

```
     !
19610 PRINT#4,"X,Y,Z",Q(1),Q(2),Q(3)
       \PRINT#4,"IO,LAM,BRANCH",IO,LAM,BR
       \PRINT#4,"THET,PHI,J",
19620 PRINT#4,57.2958*FNACS(W(3)),57.2958*ATN(W(2)/W(1)),J
       \PRINT#4,"U,V,W",W(1),W(2),W(3)
19630 PRINT#4,"I,RATIO,W2",I,RATIO,W2
       \PRINT#4,"LAY,RAD,R1",LL,Q(1)^2+Q(2)^2,Q1(1)^2+Q1(2)^2
19640 PRINT#4,"DW,DTB,DBN",DJWALL,DJTOB,DJBND
       \PRINT#4,"X',Y',Z',DJ",Q1(1),Q1(2),Q1(3),DJ
19699 PRINT#4,
       \RETURN
32373 END
```

Table A1

INPUT VARIABLE LIST

Variable	Function
ACC(10,5)	Absorption coefficients for chlorophyll a
ACP (10,5)	Absorption coefficients for subspended particulates
ACW (10,5)	Absorption coefficients for water
CONC	Concentration of chlorophyll
CONP	Concentration of particulates
CONW	Concentration of water
ETA	Fluorescent efficiency of chlorophyll a
FILE$	File name for output data storage
LO	Number of profile steps plus 1, first is always air
LAMO	Photon wavelength parameter, column index
LDPTH (10,5)	The depth of each profile step
MINW	Minimum photon weight
NEV	Number of events
NPH	Number of photons
OUT$	Output data file name
PHIO	Incident azimuth angle
RO	Random number seed
REFX (10,5)	Refractive indices of each layer
ROUT	Maximum output radius
SCC (10,5)	Scattering coefficients of chlorophyll a
SCP (10,5)	Scattering coefficients for suspended particulates
SCV$	File name for probability scattering distribution function
SCW (10,5)	Scattering coefficients of water
TANK (5,5)	External boundary parameters TANK (1,LAM)=Vertical bound radius for wavelength parameter LAM TANK (2,LAM)=Horizontal bound depth for wavelength parameter LAM TANK (3,LAM)=Vertical bound reflectivity for wavelength parameter LAM TANK (4,LAM)=Horizontal bound reflectivity for wavelength parameter LAM TANK (5,LAM)=0, (used internally)
THETØ	Incident polar angle
TITLE$	Title of output data file

The columns of multidimensional arrays represents variations in wavelength and rows (for all arrays except TANK (5,5) represent profile steps.

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