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BUCKL: A PROGRAM FOR RAPID CALCULATION
OF X-RAY DEPOSITION.

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X-RAY DEPOSITION

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ABSTRACT

A fast, analytic x-ray deposition code called BUCKL has been developed. It provides increased accuracy and versatility compared with VANDAL-F (and other exponential codes), while maintaining similar simplified input-output formats and comparable execution times. The code is believed to be sufficiently accurate for essentially all engineering calculations.

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Key word: Computer code

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BUCKL: A PROGRAM FOR RAPID CALCULATION OF X-RAY DEPOSITION

I. INTRODUCTION

There are a number of problems which require calculations of x-ray deposition in absorbing materials. For infinite one-dimensional (slab) geometry, discrete ordinates transport codes (such as DTF¹) are available, while for two-dimensional (cylindrical) problems a Monte Carlo code (such as PHOCYN²) must usually be used. For typical problems, DTF requires half a minute and PHOCYN 5 to 10 minutes (for 5- to 10-percent accuracy) for execution on the CDC 6600. In some applications, such as dosimeter design, one would like to run a large number of calculations but is limited by available computer time. In other cases, great accuracy is not required and often not justified by the data used. For these purposes fast, approximate deposition codes are very desirable, and some have been developed. The family of VANDAL³ codes are fast, though often quite inaccurate, but are limited to slab geometry. RANDAL⁴ includes an extension to finite transverse geometry and considers deposition by scattered radiation as a random walk of energy. The effect of finite transverse geometry is to reduce deposition by permitting the loss of some scattered photons through the sides of the absorber.

This report describes a fast, analytic x-ray deposition code called BUCKL, intended to provide increased accuracy and versatility in calculations where exponential codes such as VANDAL-F³ are now used. We realize that an exponential code is often quite adequate; it may also be extremely inaccurate, and the user is often unaware of the error. BUCKL has been written with input-output formats very similar to those of VANDAL-F and has comparable execution times. A typical problem requires a few seconds on the CDC 6600.

The deposition resulting from the first interaction of photons in an incident beam is truly exponential, but those photons whose first interaction is a scattering rather than photoabsorption event may deposit their energy in subsequent interactions in a decidedly nonexponential manner. It is the inability to handle this scattered energy which is responsible for the inaccuracy of all exponential codes. BUCKL evaluates the first-interaction deposition analytically. Scattered x-ray energy is then treated as a distributed source for which the deposition is calculated in diffusion approximation. If fluorescence is to be included, another diffusion calculation is performed at the fluorescence energy with the use of the appropriate fraction of the absorbed energy as a source. In the diffusion calculations, a buckling correction of the type familiar in reactor theory⁵ is included to approximate the effects of finite transverse geometry.

At first glance, one would not expect diffusion approximation to be very good for many of the problems of interest. It is often desired to know the deposition in an absorber having dimensions less than a photon mean free path, to know the deposition near a free surface, or to consider an absorber including voids. Diffusion approximation is usually considered valid only "far" from free surfaces in "large" regions (in terms of mean free paths), and it is well known to encounter difficulties in a region such as a void where streaming occurs. We note, however, that for small absorbers the deposition by scattered radiation is relatively small and need not be calculated very accurately. Further, we will find that:

1. Simple corrections may be made near free surfaces.
2. Streaming in voids may be handled outside of diffusion theory and the results "spliced in."

Finally, we note that RANDAL is really almost a diffusion code (diffusion and the random walk are very closely related) and works rather well.

BUCKL has been tested on a variety of problems to check its accuracy in comparison with other codes. Typically, its results agree with more accurate transport calculations to within 10 or 15 percent and are often better. This is true for both slab and finite transverse geometries.

Section II of this report presents the theory and derivations necessary for the BUCKL code, including diffusion approximation, longitudinal and transverse boundary conditions, treatment of fluorescence radiation, the corrections to diffusion theory to be applied at longitudinal free surfaces, and the nondiffusion-theory treatment of voids. Section III compares BUCKL results with those of VANDAL or RANDAL and of PHOCYN or DTF for a variety of problems. Sections IV and V describe BUCKL inputs and outputs, respectively. Finally, Section VI lists several of the known theoretical shortcomings of the BUCKL code and suggests how the code might be improved, should the need arise. A complete FORTRAN listing is provided in Appendix C. The code is essentially identical to a previous version⁶ of BUCKL in use at Sandia Laboratories, Albuquerque.

II. THEORY

We consider two contributions to the deposition. The first-iteration deposition is

$$D_1(x) = \rho^{-1} \sigma^{\text{abs}} I_0 \exp \left(- \int_0^x \sigma^{\text{tot}}(x') dx' \right), \quad (1)$$

attributable to photo and Compton absorption of energy from the incident beam of intensity I_0 (cal/cm²) normally incident at $x = 0$. There is an additional deposition D_2 from subsequent interactions of photons scattered out of the incident beam. It is this contribution which we will treat in diffusion approximation. The diffusion equation for the scattered energy is derived in the standard way⁷ as the P_1 approximation to the spherical harmonic expansion of the steady-state single-group transport equation

$$(\hat{\Omega} \cdot \nabla + \sigma^{\text{tot}}) f_E(\underline{r}, \hat{\Omega}) = s(\underline{r}, \hat{\Omega}) + \int f_E(\underline{r}, \hat{\Omega}') \sigma(\hat{\Omega}' \rightarrow \hat{\Omega}) d\hat{\Omega}' \quad (2)$$

Here $f_E(\underline{r}, \hat{\Omega})$ is the energy distribution function for energy at $\underline{r}$ carried by photons moving in direction $\hat{\Omega}$, and $\sigma(\hat{\Omega}' \rightarrow \hat{\Omega})$ is the scattering coefficient (in cm⁻¹, as are all of our coefficients) with the spherical harmonic expansion

$$\sigma(\hat{\Omega}' \rightarrow \hat{\Omega}) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} \sigma^{\ell} P_{\ell}(\hat{\Omega}' \cdot \hat{\Omega}) \quad (3)$$

The term s is a source term representing energy scattered out of the incident beam, which is given by

$$s(\underline{r}, \hat{\Omega}) = \sigma(\hat{k} \rightarrow \hat{\Omega}) I_0 \exp \left(- \int_0^x \sigma^{\text{tot}}(x') dx' \right), \quad (4)$$

where $\hat{k}$ is a unit vector in the direction of the beam. We make the P_1 approximation by taking the distribution function to be

$$f_E(\underline{r}, \hat{\Omega}) = (4\pi)^{-1} [\epsilon(\underline{r}) + 3\hat{\Omega} \cdot \underline{J}(\underline{r})], \quad (5)$$

where ϵ is the energy density and $\underline{J}$ the energy current. Substituting

Eq. (5) into Eq. (2) and projecting out the first two multipole components gives (after eliminating $\tilde{J}$ from the P_0 equation) equations resembling familiar diffusion theory:

$$\tilde{J} = - (3\sigma_d^{\text{tr}})^{-1} \nabla \cdot \epsilon + (\sigma_d^{\text{tr}})^{-1} \sigma^1 \hat{k} I_0 \exp \left(- \int_0^x \sigma^{\text{tot}}(x') dx' \right), \quad (6)$$

$$(\kappa_0^2 - \nabla^2) \epsilon = S. \quad (7)$$

Here

$$\sigma^{\text{tr}} \equiv \sigma^{\text{tot}} - \sigma^1 \quad (8)$$

is the transport coefficient, and

$$\kappa_0 = (3\sigma_d^{\text{abs}} \sigma_d^{\text{tr}})^{1/2} \quad (9)$$

is the inverse diffusion length. The meaning of the d's will be made clear later. Finally, the diffusion source term S is

$$S = 3I_0 (\sigma^0 \sigma_d^{\text{tr}} + \sigma^1 \sigma^{\text{tot}}) \exp \left(- \int_0^x \sigma^{\text{tot}}(x') dx' \right). \quad (10)$$

Most treatments of diffusion theory assume an isotropic source, and would lead one to write Eq. (10) without the σ^1 term, which arises from the anisotropy of our source. This term is present for our problem and is rather important at high photon energies.

We emphasize that all of our σ coefficients are for absorption and scattering of energy, not of photons. Thus σ^{abs} contains both photo and Compton-absorption contributions, and the isotropic scattering coefficient is

$$\sigma^0 = \sigma^{\text{tot}} - \sigma^{\text{abs}} \quad (11)$$

rather than $\sigma^{\text{tot}} - \sigma^{\text{photo}}$. BUCKL obtains σ^{tot} and σ^{abs} from Biggs-Lighthill analytic fits,⁸ using coefficients stored on the VANDAL data tape. Equation (11) then gives σ^0 from which σ^1 may be obtained. The ratio σ^1/σ^0 is a universal function of photon energy which we calculate in the following manner.

The energy scattering cross section is related to the Klein-Nishina cross section by

$$\left(\frac{d\sigma}{d\Omega} \right)_E = \frac{h\nu'}{h\nu} \left(\frac{d\sigma}{d\Omega} \right)_{K-N} , \quad (12)$$

where $h\nu'$ is the energy of the scattered photon. In terms of the variable α ,

$$\alpha \equiv \frac{h\nu}{m_e c^2} , \quad (13)$$

which is simply the photon energy in units of the rest mass of an electron, and we have

$$\frac{h\nu'}{h\nu} = \frac{1}{1 + \alpha(1 - \cos \theta)} , \quad (14)$$

where θ is the scattering angle. The multipole components are given by

$$\sigma^\ell = \int \left(\frac{h\nu'}{h\nu} \frac{d\sigma}{d\Omega} \right)_{K-N} P_\ell(\cos \theta) d\Omega , \quad (15)$$

where the Klein-Nishina cross section is given by

$$\begin{aligned} \left(\frac{d\sigma}{d\Omega} \right)_{K-N} &= \frac{3}{16\pi} \sigma_{Th} \frac{1 + \cos^2 \theta}{[1 + 2\alpha \sin^2(\theta/2)]^2} \cdot \\ &\cdot \left\{ 1 + \frac{4\alpha^2 \sin^4(\theta/2)}{(1 + \cos^2 \theta) [1 + 2\alpha \sin^2(\theta/2)]} \right\} , \end{aligned} \quad (16)$$

with σ_{Th} the Thomson cross section. Following Renken,⁹ we change the integration variable to α' , and write

$$\begin{aligned} \sigma^\ell &= \frac{3}{8} \sigma_{Th} \int_{\alpha/(1+2\alpha)}^{\alpha} \left(\frac{\alpha'}{\alpha} \right)^3 \left\{ \frac{\alpha}{\alpha'} + \frac{\alpha'}{\alpha} - 2 \left[\frac{1}{\alpha'} - \frac{1}{\alpha} \right] + \left[\frac{1}{\alpha'} - \frac{1}{\alpha} \right]^2 \right\} \cdot \\ &\cdot P_\ell \left(1 + \frac{1}{\alpha} - \frac{1}{\alpha'} \right) \frac{d\alpha'}{\alpha'^2} . \end{aligned} \quad (17)$$

This leads to

$$\sigma^0 = \frac{3}{8} \frac{\sigma_{Th}}{\alpha^3} \left\{ \ln(1 + 2\alpha) + \frac{2\alpha(4\alpha^2 - 3\alpha - 3)}{3(1 + 2\alpha)} + \frac{4\alpha^3(1 + \alpha)}{3(1 + 2\alpha)^2} \right\}, \quad (18)$$

$$\sigma^1 = \left(1 + \frac{1}{\alpha}\right) \sigma^0 - \frac{3}{8} \frac{\sigma_{Th}}{\alpha^3} \left\{ \left(\alpha - 2 - \frac{2}{\alpha}\right) \ln(1 + 2\alpha) + 4 + \frac{2\alpha^2(1 + \alpha)}{(1 + 2\alpha)^2} \right\}. \quad (19)$$

A 1-percent fit to the ratio is given by

$$f_{1E} \equiv \frac{\sigma^1}{\sigma^0} \approx \frac{2.35 \times 10^{-3} h\nu}{1 + 2.9826 \times 10^{-3} h\nu + 4.8537 \times 10^{-8} (h\nu)^2 + 1.04317 \times 10^{-9} (h\nu)^3} \quad 0 \leq h\nu \leq 800 \text{ keV} \quad (20)$$

for the photon energy $h\nu$ in keV. This function is shown in Fig. 1. This and others used by BUCKL are least-square fits for which the techniques of Biggs¹⁰ are used.

Fig. 1 Ratio of P_1 to P_0 coefficients for Compton scattering.

The scattered photons which make up the energy density ϵ have been degraded in energy by Compton scattering. If this is considered, it may be seen that some of the coefficients in Eqs. (6), (8), (9), and (10), those which have been labeled by a subscript d, should be evaluated at some average degraded energy (which we shall take to be the average energy of a once-scattered photon) rather than at the beam energy.

The average degraded energy is easily obtained from the Klein-Nishina equation. Values were obtained from the tables given by Biggs, which are fit to 0.1 percent by

$$\frac{h\nu'}{h\nu} = \frac{1 + 2.6258 \times 10^{-3} h\nu}{1 + 4.5543 \times 10^{-3} h\nu + 9.3131 \times 10^{-7} (h\nu)^2} \quad (21)$$

$$0 \leq h\nu \leq 1000 \text{ keV}$$

for the energy $h\nu$ in keV. This function is shown in Fig. 2. We see that energy degradation may be rather important: The average energy loss of a scattered 100-keV photon is about 14 keV.

Fig. 2 Average energy of Compton-scattered photons.

The average deposition by scattered photons is then

$$D_2(x) = \rho^{-1} \sigma_d^{\text{abs}} \epsilon_{\text{av}}(x) , \quad (22)$$

where $\epsilon_{\text{av}}(x)$ is $\epsilon(\tilde{r})$ averaged over the transverse area.

The solution to the homogeneous ($S = 0$) diffusion, Eq. (17), in cylindrical coordinates r, x is

$$\epsilon(\tilde{r}) = (B e^{-\kappa x} + C e^{\kappa x}) J_0(kr) , \quad (23)$$

$$\kappa^2 = \kappa_0^2 + k^2 , \quad (24)$$

where J_0 is the Bessel function of order zero and k is to be chosen to satisfy a boundary condition at the transverse free surface as discussed below. If we assume (as is usually done) that the J_0 transverse dependence applies to S also, the complete solution to Eq. (7) is (averaged over r)

$$\epsilon_{\text{av}}(x) = \frac{S(x)}{\kappa^2 - (\sigma^{\text{tot}})^2} + B e^{-\kappa x} + C e^{\kappa x} \quad (25)$$

in any homogeneous region. The B and C must be chosen to match boundary conditions at free surfaces or at interfaces with other materials, as will be described below.

Since κ may equal σ^{tot} , the appearance of $\kappa^2 - (\sigma^{\text{tot}})^2$ in the denominator of Eq. (25) might lead to difficulties. However, we note that S behaves locally as $\exp(-\sigma^{\text{tot}}x)$ (see Eq. (6) and, since $\kappa \rightarrow \sigma^{\text{tot}}$, this divergent term will be nearly cancelled by the $\exp(-\kappa x)$ term. The sum remains finite (to satisfy boundary or matching conditions at the ends), picking up a term proportional to $x \exp(-\kappa x)$ in the limit. In order to prevent calculational difficulties, BUCKL prevents the denominator from being less than $10^{-4} \kappa^2$ in magnitude; physically, this may be thought of as making a very slight change in the diameter of the absorber.

Longitudinal Boundary Conditions

At an interface with another material, the proper boundary condition is continuity of $f_E(\underline{r}, \underline{\Omega})$ across the interface. In diffusion approximation we match ϵ and $\underline{J}$ (see Eq. (5); in fact, we have only enough freedom to match ϵ and $\underline{J} \cdot \hat{x}$. In Eq. (6), $\underline{J}$ is the sum of two terms,

$$\underline{J}_1 = - \left(3\sigma_d^{\text{tr}} \right)^{-1} \nabla \epsilon, \quad (26)$$

associated with the diffusing energy and a second term which arises solely from the anisotropy of the scatter source. We feel that it is $\underline{J}_1 \cdot \hat{x}$ which should be continuous.

Equivalently, we may require continuity of the two "directed currents" defined by

$$I_{\pm} = \int_{\mu \gtrless 0} d\Omega \, \underline{\Omega} \cdot \hat{x} f_E(\underline{r}, \underline{\Omega}) = \frac{1}{4} \left(1 \mp \Delta \frac{\partial}{\partial x} \right) \epsilon_{av}(x), \quad (27)$$

diffusion

where $\Delta = \frac{2}{3\sigma_d^{\text{tr}}}$. The value $I_{\pm}$ has the interpretation of energy passing to the $\left(\begin{smallmatrix} \text{right} \\ \text{left} \end{smallmatrix} \right)$ through a unit area normal to $\hat{x}$.

At a free surface, the exact boundary condition of no incoming photons must be replaced by the approximate Marshak boundary condition¹¹ of no incoming current. That is, we require

$$I_{\pm} \big|_{\text{surface}} = 0 \quad \text{at} \quad \left(\begin{smallmatrix} \text{left} \\ \text{right} \end{smallmatrix} \right) \text{ free surface.} \quad (28)$$

In slab geometry this problem, the "Milne Problem," may be solved exactly¹² (with certain simplifying restrictions), and gives, for a scattering medium,

$$\Delta \approx 0.71 \left(\sigma_d^{\text{tr}} \right)^{-1}, \quad (29)$$

which we shall assume to hold in general. Δ is called the "extrapolation distance" and is the distance at which ϵ extrapolates to zero.

Transverse Boundary Condition

For large cylinders, the Milne boundary condition must hold on the lateral surface also, with

$$\left(1 + \Delta \frac{1}{r} \frac{\partial}{\partial r} r\right) \epsilon(r) \Big|_{r=R} = 0, \quad (30)$$

which leads to $J_0(kR) + k \Delta J_1(kR) = 0$, or

$$k \approx \frac{2.405}{R+\Delta} \equiv \frac{2.405}{R^*}, \quad (31)$$

where 2.405 is the first zero of $J_0(x)$ and R^* is called the extrapolated radius.

For small cylinders ($\sigma^{\text{tr}} R \ll 1$), this boundary condition and, in fact, diffusion theory itself is invalid. We may, however, solve the transport equation exactly in this limit and pick R^* such that the formalism outlined above gives the correct answer.

For a small cylinder ($\sigma^{\text{tot}} R \ll 1$), ϵ is made up almost entirely of once-scattered photons, most of which escape through the lateral surface of the cylinder without further interactions. Thus we may compute $\epsilon(\underline{x})$ by summing the contributions of photons scattered at various points in the cylinder, weighted by the probability that they will arrive at $\underline{x}$ without further interaction. The integrals are straightforward and give, after averaging over the cross sectional area,

$$\epsilon(\underline{x}) = \frac{4}{3} \sigma^0 R I_0 \exp\left(-\int_0^x \sigma^{\text{tot}}(x') dx'\right) [1 + O(\sigma^{\text{tot}} R)]. \quad (32)$$

From the formalism above, we find

$$\epsilon(\underline{x}) = 3 \left(\frac{\sigma^0 \sigma_d^{\text{tr}} + \sigma^1 \sigma^{\text{tot}}}{\kappa^2} \right) I_0 \exp\left(-\int_0^x \sigma^{\text{tot}}(x') dx'\right) \left[1 + O\left(\frac{\sigma^{\text{tot}}}{\kappa}\right) \right] \quad (33)$$

in this limit, since $\kappa \rightarrow \infty$ and B and C are of order $\left(\frac{\sigma^{\text{tot}}}{\kappa}\right)^3$.

Then

$$\begin{aligned}
k^2 &= \left(\frac{2.405}{R^*} \right)^2 = \kappa^2 \left[1 + 0 \left(\left(\frac{\sigma^{\text{tot}}}{\kappa} \right)^2 \right) \right] \\
&= \frac{9}{4} \frac{\sigma^0 \sigma_d^{\text{tr}} + \sigma^1 \sigma^{\text{tot}}}{\sigma^0 R} \left[1 + 0 \left(\frac{\sigma^{\text{tot}}}{\kappa} \right) \right]. \quad (34)
\end{aligned}$$

And finally,

$$\sigma_d^{\text{tr}} R^* = 1.6 \left(\sigma_d^{\text{tr}} R \right)^{\frac{1}{2}} \left[1 + 0 \left(\left(\sigma_d^{\text{tr}} R \right)^{\frac{1}{2}} \right) + 0 \left(\frac{\sigma^1}{\sigma^0} \right) \right]. \quad (35)$$

In this limit, ϵ and D_2 will be small, and great accuracy is not required in their calculation. Therefore, we will take

$$R^* \xrightarrow{R \rightarrow 0} 1.6 \left(\frac{R}{\sigma_d^{\text{tr}}} \right)^{1/2}, \quad (36)$$

where we have neglected $\frac{\sigma^1}{\sigma^0}$ compared to 1, a good approximation except at very high energies. In Fig. 3 we plot $\sigma_d^{\text{tr}}(R^* - R)$ against $\sigma_d^{\text{tr}}R$ in both limits and also a simple function which is a reasonable fit in both limits and provides a smooth interpolation between. This approximate fit,

$$\sigma_d^{\text{tr}} (R^* - R) \approx 0.71 - \left(0.49 e^{-5\sigma_d^{\text{tr}} R} + 0.22 e^{-40\sigma_d^{\text{tr}} R} \right), \quad (37)$$

has been used in the computer code.

In a problem containing n homogeneous layers, Eqs. (24), (31), and (37) fix κ for each layer. The boundary conditions (continuity of $I_{\pm}$) provide $2n$ equations (one at each of the two free surfaces, two at each of the $n-1$ interfaces) in $2n$ unknowns (n B 's and n C 's; see Eq. (25)). The BUCKL code solves this system of linear equations (once for each energy group) to find an analytic expression for the density (and therefore the deposition) which is then evaluated wherever the deposition is desired.

Fig. 3 Extrapolated radius as a function of physical radius.

Correction at Longitudinal Free Surfaces

It is well known that diffusion approximation gives the wrong results near free surfaces, and the boundary conditions we have used are those which lead to correct results deep inside the material. In the classical Milne case (no incident flux, no sources) the density falls off near the surface from the diffusion theory result by a factor which is a universal function of the depth in free paths.

It seems reasonable to expect that a similar result might obtain, at least approximately, in our case. The presence of volume sources (scattering out of the main beam) and of a distinguished direction (the beam direction) suggests that the appropriate reduction factor should be different from the Milne case, and possibly different for the two ends.

These factors have been determined empirically. The ratio between DTF or PHOCYN results and BUCKL results for D_2 , the additional deposition by scattered photons, was calculated as a function of depth in (transport) free paths for a number of cases. The scatter was not great, typically

about 5 percent, and a simple fit to the consensus was made, giving

$$\frac{D_2(\text{PHOCYN})}{D_2(\text{diffusion})} \approx \begin{cases} 1.0 - 0.28 \exp(-10\sigma^{\text{tr}} |x - x_{\text{end}}|) & \text{(end facing source)} \\ 1.0 - 0.18 \exp(-7.3\sigma^{\text{tr}} |x - x_{\text{end}}|) & \text{(end away from source)} \end{cases} \quad (38)$$

These fits are shown in Fig. 4, together with the Milne problem results for comparison.

The BUCKL code simply multiplies the additional deposition D_2 by these surface-reduction factors before adding it to D_1 to get the total deposition, and assumes that they are independent, even for short absorbers.

Fig. 4 Correction factors at free surfaces.

Voids

Many practical problems involve absorbers with voids, i.e., layers containing no material. For slab geometry, these voids have no effect on deposition and may be ignored. For absorbers with finite transverse dimensions, however, energy will be lost out the sides: Photons entering the void from material on one side may miss the material on the other side.

Marshak boundary conditions¹¹ for a void extending from x_L to x_R require

$$\left[1 - \frac{2}{3\sigma_d \text{tr}} \frac{\partial}{\partial x} \right] \epsilon \Big|_{x_R} = 4 \int d\tilde{\Omega} \mu T(\tilde{\Omega}) , \quad (39)$$

where $T(\tilde{\Omega})$ is the incident distribution at x_R . For a finite radius we will average over the cross-sectional area.

The distribution at x_L is, in diffusion approximation and neglecting the variation with radius,

$$f(\tilde{\Omega}) \Big|_{x_L} = \frac{1}{4\pi} \left(1 - \frac{1}{\sigma_d \text{tr}} \mu \frac{\partial}{\partial x} \right) \epsilon \Big|_{x_L} . \quad (40)$$

Since photons undergo no interactions in traversing the void, we have simply

$$T(\tilde{x}, \tilde{\Omega}) = \begin{cases} f(\tilde{\Omega}) \Big|_{x_L} & \text{if the line through } \tilde{x} \text{ in direction } \\ & - \tilde{\Omega} \text{ intersects the surface at } x_L \\ 0 & \text{otherwise} \end{cases} . \quad (41)$$

A little thought will show that what we are really doing is requiring continuity of I_+ (see Eq. (27)) but using P_1 transport theory in the void rather than diffusion theory. This analysis leads to the boundary condition for the energy density (again replacing $\frac{2}{3\sigma \text{tr}}$ by Δ):

$$\left(1 - \Delta \frac{\partial}{\partial x} \right) \epsilon \Big|_{x_R} = \left[F_1 \left(\frac{L}{R} \right) - F_2 \left(\frac{L}{R} \right) \Delta \frac{\partial}{\partial x} \right] \epsilon \Big|_{x_L} , \quad (42)$$

and a similar condition at x_L :

$$\left(1 + \Delta \frac{\partial}{\partial x} \right) \epsilon \Big|_{x_L} = \left[F_1 \left(\frac{L}{R} \right) + F_2 \left(\frac{L}{R} \right) \frac{\partial}{\partial x} \right] \epsilon \Big|_{x_R} , \quad (43)$$

where $L \equiv x_R - x_L$ is the length of the void, and

$$F_{1,2} = 2 \int_{[1 + 4R^2/L^2]^{-1/2}}^1 G\left(\mu, \frac{L}{R}\right) \mu^{1,2} d\mu \quad . \quad (44)$$

The lower limit of integration is the least value of μ with which a photon can cross the void, and

$$G\left(\mu, \frac{L}{R}\right) = H\left(\sqrt{\frac{1 - \mu^2}{\mu}} \frac{L}{R}\right) \quad , \quad (45)$$

with

$$H(x) = \begin{cases} (1 - x^2)^{1/2} + \frac{2}{\pi} \int_{1-x}^1 \cos^{-1}\left(\frac{s^2 + x^2 - 1}{2sx}\right) s ds; & 0 \leq x \leq 1 \\ \frac{2}{\pi} \int_{x-1}^1 \cos^{-1}\left(\frac{s^2 + x^2 - 1}{2sx}\right) s ds; & 1 \leq x \leq 2 \end{cases} \quad . \quad (46)$$

Geometrically, $H(x)$ is just the fraction of the circumference of a circle of radius x which lies inside the unit circle, averaged over the position of its center inside that unit circle.

A numerical integration of Eq. (46) and then of Eq. (44) produced the curves shown in Fig. 5, which are probably accurate to 1 or 2 percent. These are fit to about 1 percent by

$$F_1(x) = \frac{1 + 0.2271x}{1 + 1.0672x + 0.8133x^2 + 0.2271x^3} \quad , \quad (47)$$

$$F_2(x) = \frac{1 + 0.13182x}{1 + 0.5930x + 0.5651x^2 + 0.08788x^3} \quad , \quad (48)$$

and these fits are used in BUCKL. Note that two consecutive voids are not equivalent to a single void in this formulation because $F_i\left(\frac{L_1}{R}\right)F_i\left(\frac{L_2}{R}\right) \neq F_i\left(\frac{L_1 + L_2}{R}\right)$: Mathematically, transmission across a void does not have the group property. BUCKL prevents any attempt to specify two adjacent voids.

Fig. 5 Transmission factors for voids.

Fluorescence

If energy is deposited by photons of energy $h\nu$ in an absorber which contains element Z with weight fraction W_Z , a fraction $W_Z \sigma_Z^{\text{ph}} / \sigma^{\text{abs}}$ of that energy will be absorbed by photo events in Z atoms. Here σ^{abs} is the energy absorption coefficient of the possibly composite material, and it is obtained as a weighted sum of the coefficients for the constituent elements. If $h\nu$ is above the K (or L) absorption edge for element Z, a fraction $f_{K(L)}$ of these photo events will produce a K(L) vacancy, and a fraction $w^{K(L)}$ of these vacancies will be de-excited with emission of a K(L) fluorescence photon of mean energy $h\nu_{K(L)}$. We therefore have a distributed isotropic source of energy at $h\nu_{K(L)}$ with intensity

$$S_{F\ell}(x) = \rho^{-1} D(x) W_Z \sigma_Z^{\text{ph}} (\sigma^{\text{abs}})^{-1} f_{K(L)} w^{K(L)} \frac{h\nu_{K(L)}}{h\nu}, \quad (49)$$

where S is in energy /cm³ and D is the total prefluorescence deposition in energy/gm.

We treat this energy in diffusion approximation exactly in the same manner as for scattered energy, and solve

$$(\kappa^2 - \gamma^2) \epsilon_{F\ell} = S_{F\ell}(x) \quad , \quad (50)$$

with κ evaluated at the mean fluorescence energy $h\nu_{K(L)}$. The particular solution is not so simple now (S is not exponential), but if we can construct one, the general solution is

$$\epsilon_{F\ell} = \epsilon_{F\ell}^{\text{particular}} + B e^{-\kappa x} + C e^{\kappa x} \quad , \quad (51)$$

where B and C are chosen to satisfy boundary conditions exactly as before. At the time that fluorescence is considered, BUCKL has a table of values of $S_{F\ell}(x)$ at various points, resulting from fluorescence excited by the incident spectrum and perhaps by other fluorescence lines of sufficiently great energy (refluorescence). The problem is to find a particular solution. We know $S_{F\ell}$ at two adjacent points x_i and x_{i+1} , and we assume that between these points $D(x)$ is reasonably fit by an exponential. A particular solution is then simply given by

$$\epsilon_{F\ell}^{\text{particular}}(x) \Big|_{x \text{ in } N^{\text{th}} \text{ homogeneous layer}} = \sum_{x_{i,i+1} \text{ in } N^{\text{th}} \text{ layer}} q_{i,i+1}(x) \quad , \quad (52)$$

where $q_{i,i+1}(x)$ is the solution resulting from sources between x_i and x_{i+1} given by

$$q_{i,i+1}(x) = \begin{cases} c_\ell e^{\kappa(x-x_i)} & x \leq x_i \\ (\kappa^2 - \gamma^2)^{-1} S_{F\ell}(x) & x_i \leq x \leq x_{i+1} \\ + c e^{\kappa(x-x_i)} + b e^{\kappa(x_{i+1}-x)} & \\ b_r e^{\kappa(x_{i+1}-x)} & x \geq x_{i+1} \end{cases} \quad , \quad (53)$$

where the b 's and c 's are chosen to satisfy continuity of $I_\pm$ (Eq. (27)) at x_i and x_{i+1} , and $S_{F\ell}$ has been approximated by

$$S_{F\ell}(x) \approx S_{F\ell}(x_i) e^{-\gamma(x-x_i)} \quad , \quad x_i \leq x \leq x_{i+1} \quad . \quad (54)$$

Straightforward algebra gives

$$\begin{aligned} c_\ell &= q_{i,i+1}(x_i) = \frac{3}{2} \rho \sigma^{\text{tr}} \kappa^{-1} (\kappa + \gamma)^{-1} S_{F\ell}(x_i) (1 - e^{-\gamma\delta} e^{-\kappa\delta}) , \\ b_r &= q_{i,i+1}(x_{i+1}) = \frac{3}{2} \rho \sigma^{\text{tr}} \kappa^{-1} (\kappa - \gamma)^{-1} S_{F\ell}(x_{i+1}) (1 - e^{\gamma\delta} e^{-\kappa\delta}) , \end{aligned} \quad (55)$$

where $\delta = x_{i+1} - x_i$. BUCKL uses Eqs. (52) through (55) to construct a particular solution for a given fluorescence line, and then completes the general solution (51) exactly in the same manner as for scattered energy.

We emphasize here a significant difference from the treatment of fluorescence in VANDAL-F.³ VANDAL-F constructs $\epsilon_{F\ell}$ by superimposing solutions for sources in each interval $x_i \leq x \leq x_{i+1}$, using a transport solution based on the exponential integral. With VANDAL-F, one never worries about boundary conditions other than continuity of ϵ . In this superposition, however, it is assumed that all fluorescence photons start at the zone center $\frac{1}{2}(x_i + x_{i+1})$. If, through an unfortunate choice of zoning, $\frac{1}{2}(x_{i+1} - x_i)$ is several mean free paths at $h\nu_{F\ell}$, very few fluorescence photons will reach x_i or x_{i+1} to be counted. The effect is that some fraction, perhaps essentially all, of the fluorescence energy in a VANDAL-F calculation can disappear without trace. BUCKL, however, has the correct behavior in this limit, with

$$\epsilon_{F\ell}(x) \xrightarrow[\kappa \delta x \rightarrow \infty]{} \rho (\sigma^{\text{abs}})^{-1} S_{F\ell}(x) . \quad (56)$$

BUCKL requires values for the fluorescence parameters $h\nu_{F\ell}$, f_K , f_L , ω^K , ω^L . The usual assumption is made that f_K is independent of energy above the K absorption edge, and that f_L is constant between the L and K edges and is reduced by the constant factor $(1 - f_K)$ above the K edge. Internal analytic fits are supplied to compute these parameters as a function of Z , but the user can supply his own values to override these fits if desired. The term f_K is evaluated as

$$f_K = (\sigma_{K+}^{\text{ph}} - \sigma_{K-}^{\text{ph}}) / \sigma_{K+}^{\text{ph}} , \quad (57)$$

where $K^\pm$ means that the parameter is evaluated just above or below the K edge, and f_L is evaluated similarly. The Los Alamos¹³ compilation of data is used for $h\nu_{F\ell}$, f_K and f_L , and the recent extensive review article by Fink et al.¹⁴ for ω^K and ω^L .

The fits used by BUCKL are:

$$h\nu_{F\ell,K} = (6.7527 \times 10^{-3} + 7.5653 \times 10^{-6} Z - 1.72367 \times 10^{-7} Z^2 + 2.0019 \times 10^{-9} Z^3) Z^{2.104}, \quad (58)$$

$$h\nu_{F\ell,L} = (1.35427 \times 10^{-4} - 1.13774 \times 10^{-7} Z - 8.8858 \times 10^{-9} Z^2 + 6.2853 \times 10^{-11} Z^3) Z^{2.6458}, \quad (59)$$

$$f_K = 0.957 - 2.51 \times 10^{-3} Z + 6.0 \times 10^{-6} Z^2, \quad (60)$$

$$f_L = 1.000 - 4.42 \times 10^{-3} Z + 1.967 \times 10^{-5} Z^2, \quad (61)$$

$$\omega^K = (0.9463 + (18.045/Z)^2)/(1.0 + (35.374/Z)^4), \quad (62)$$

$$\omega^L = \begin{cases} -0.199 + 0.00621 Z & 40 \leq Z < 70 \\ (2.08 + (75.5/Z)^{10})^{-1} & Z \geq 70 \end{cases}. \quad (63)$$

These functions are plotted in Figs. 6, 7, and 8. It is believed that these fits are as accurate as the experimental data justifies in the ranges of $Z \geq 15$ for K fluorescence and $Z \geq 40$ for L fluorescence. For smaller Z numbers, the fluorescence efficiencies $\omega^{K,L}$ are less than about 5 percent, and BUCKL neglects fluorescence effects.

Fig. 6 Mean K and L fluorescence energies.

Fig. 7 Fit to K and L jump ratios.

Fig. 8 Fit to K and L fluorescence efficiencies.

III. COMPARISON WITH OTHER CODES

In order to check the various approximations and assumptions used in BUCKL, we have made a number of comparisons with more exact codes, DTF and PHOCYN, and also with RANDAL.

The first case considered is deposition by monoenergetic 100-keV photons in pure aluminum. DTF or PHOCYN, BUCKL, and RANDAL results are shown in Fig. 9 for cylinders 10 cm long and with various radii, and in Fig. 10 for slabs 1 and 3 cm thick. BUCKL is seen to agree with the more exact codes to about 10 percent. PHOCYN was run to a precision of about 5 percent in general and to about 1 percent for the 2-cm radius. RANDAL is somewhat less accurate, particularly at the larger radii.

Fig. 9 Deposition at 100 keV in pure aluminum cylinders.

Fig. 10 Deposition at 100 keV in pure aluminum slabs.

In the course of these comparisons it was discovered that, in the development of RANDAL, radius and diameter had occasionally been interchanged. When this was corrected it was found that agreement was markedly better if the "average lateral dimension" in RANDAL was interpreted as radius rather than diameter. This change has been made in RANDAL and accounts for the differences between our Figs. 9 and 11, and Figs. 2 through 5 of the RANDAL report.

Also shown, strictly for comparison, are two VANDAL-type results, $\rho^{-1} \sigma^{abs} \exp(-\sigma^{tot}x)$ (which corresponds to the $R = 0$ case) and $\rho^{-1} \sigma^{abs} \exp(-\sigma^{abs}x)$. Both are seen to err greatly, in many cases by as much as a factor of 10.

The next case considered was a cylinder of polyethylene, 2.5 cm in diameter and 2.8 cm in length, with incident monoenergetic 20-, 30-, or 60-keV photons. Results are shown in Fig. 11 where the additional deposition D_2 is plotted. For these cases, D_2 is 10 to 20 or 25 percent of the first interaction deposition D_1 . The error bars correspond to the error in D_2 , which would produce an error of ± 5 percent in the total deposition. BUCKL and RANDAL are in very good agreement with each other and within about 6 percent, in total deposition, of PHOCYN.

Fig. 11 Deposition at 20, 30, and 60 keV in polyethylene cylinders.

A number of tests of the fluorescence part of BUCKL were conducted. Typical of them is the test problem contained in the DTF report,¹ in which photons with a spectrum of $1 \text{ photon/cm}^2/\text{keV}$ in the range $25.88 \leq h\nu \leq 40.00 \text{ keV}$ are incident on an absorber consisting of three layers:

0.006 cm Ag_3SbS_3	,	5.76 gm/cm ³	,
0.008 cm S	,	1.96 gm/cm ³	,
0.006 cm SnTe	,	6.48 gm/cm ³	.

DTF and BUCKL results are shown in Fig. 12, with and without consideration of fluorescence effects from Ag, Sb, Sn, and Te. The fluorescence parameters used in the DTF report were used and depositions normalized.

A final set of examples was calculated to check fluorescence, matching between layers, and transmission across voids. The problem considered was 100-keV monoenergetic photons incident on 3 cm of aluminum, followed by 0.03 cm of gold, followed by another 3 cm of aluminum.

Fig. 12 Deposition for the DTF report test problem.

The results for slab geometry are shown in Fig. 13, where BUCKL results may be seen to be in good agreement with those of DTF. Results from VANDAL and VANDAL-F, on the other hand, differ considerably from transport results.

Fig. 13 Deposition in an Al/Au/Al sandwich slab.

To show the effects of finite transverse geometry and of transmission across voids, the calculations were rerun for a diameter of 2 cm. Two cases were considered: one with the layers in contact, the other with 5-cm voids between the layers. Results are shown in Fig. 14, where the slab geometry result is reproduced for comparison. One can see the significant reduction in deposition caused by transverse loss of photons

and the additional reduction produced when the layers are separated. This latter reduction is primarily attributable to loss of those fluorescence photons from the gold which miss the aluminum, i.e., to solid angle effects. The agreement with PHOCYN is good. It should be mentioned that it proved impossible to calculate this problem directly with PHOCYN: The finite size of the tables used by PHOCYN resulted in no first interactions in some zones. We therefore used only the deposition from higher order interactions and added in the analytic first-interaction term.

Fig. 14 Deposition in an Al/Au/Al sandwich cylinder.

IV. DESCRIPTION OF PROGRAM SETUP

Several problems may be run sequentially, and one need not respecify parts of the problem which are unchanged.

BUCKL requires the VANDAL data tape equipped as TAPE15 and a plot tape (if used) equipped as TAPE40.

The following input data elements are required:

1. An integration range card: EMIN, DE, EMAX, PUNCH, FLUOR, PRNT, PLOT, FATAL, in FORMAT (3F8.0, 8X, F8.0, 8X, 4F8.0).

Deposition will be calculated for energies between EMIN and EMAX (EMIN if $EMAX \leq EMIN$) with trapezoid rule integration and an integration increment of DE (0.1 if $DE \leq 0$), unless these are changed by the spectrum deck. (All energies are in keV.)

If FLUOR is nonzero, the fluorescence option will be chosen (this is in the VANDAL-F IZFL field).

PRNT and PLOT are flags which, if nonzero, will suppress the printed and plotted outputs, respectively. (These are in previously unused fields. The VANDAL-F PRNT field is not read, and printed output is now the default option.)

If BUCKL encounters certain difficulties, such as a spectrum not locatable on tape or a problem which exceeds maximum array dimensions, it will discontinue execution of that problem and search on through the data for a NEXTJOB deck, unless the flag FATAL is nonzero, in which case EXIT will be called.

2. A spectrum deck in one of four forms.

- A. A weighted sum of up to 50 blackbodies. The first card has a B in Column 1. Starting with the second card, NBB (number of blackbodies) and NBB pairs of W(I) (relative weight, need not be normalized) and T(I) (temperature in keV) are listed in FORMAT (I10, 7F10.5/ (8F10.5)). For this option, if EMIN, DE, and EMAX are left blank on the range card, the program will calculate an appropriate range.

B. A spectrum tabulated at the integration points. The first card contains an S in Column 1, and the format for the ordinate values in Columns 9 to 16. Starting with the second card, ordinate values at $EMIN + DE * I$ are listed in the specified format.

C. An arbitrarily tabulated spectrum. The first card contains S/E in Columns 1 to 3, a format in Columns 9 to 16, and NSEG, the number of tabulated spectral points as an integer, in Columns 17 to 24. Starting with the second card, there are listed NSEG energy values and, starting a new card, NSEG intensities, all in the specified format. The program linearly interpolates in this segmented spectrum to obtain spectral values at the integration points from EMIN to EMAX.

D. A spectrum stored on Tape 15 may be used by calling the proper spectrum name, starting in Column 1. In this case EMIN, DE, and EMAX will be respecified from data on the tape.

3. A fluence card, with the incident fluence in cal/cm^2 in FORMAT (F8.0).

4. A title card, containing up to 80 characters to be printed as a title on both the plots and the printed output.

5. A fluorescer deck, if the flag FLUOR is nonzero. The first card contains NZF, the number of fluorescence "lines" in FORMAT (I4). NZF must not exceed 10. This card is followed by NZF cards, one for each fluorescence line (in any order), each containing IZ, EFL, YIELDK, JUMPK, YIELDL, JUMPL in FORMAT (I4, 5F10.4). IZ is plus or minus the Z number of the fluorescing element, plus for K fluorescence, minus for L fluorescence. If it is desired to consider both K and L fluorescence from a single element IZ two cards will be required, one with IZ and one with - IZ. The remaining fields are optional: BUCKL will supply any of the necessary fluorescence parameters which are not specified by the user and will print the values used. These are the mean line energy, the K yield, the K jump ratio (fraction of the photo cross section at the K edge which is due to K absorption), the L yield, and the L jump ratio.

BUCKL will not compute the effects of K(L) fluorescence from elements with Z less than 15 (40). Data for such fluorescence lines may be included, but they will be ignored, as will data for any element not present in the absorber. Thus, one can run a no-fluorescence calculation with FLUOR nonzero if desired.

6. A diameter card, giving the stack diameter in cm in FORMAT (F10.0).

7. A material deck, with two cards for each homogeneous layer. The cards contain

XTHICK, RHO, NOZ, NSHELLS - FORMAT (2F8.0, 2I5)
(NZZ(I), W(I), I = 1, NOZ) - FORMAT (8(I2,F8,0))

for a layer of thickness XTHICK (cm) and density RHO (gm/cm^3) containing NOZ elements with atomic numbers NZZ(I) and (unnormalized) weight fractions W(I). Deposition will be calculated at NSHELLS + 1 equally spaced points, including the front and back of the layer.

Pairs of cards, one pair for each homogeneous layer, are repeated until the absorber has been completely specified.

A BLANK CARD must be included after the last pair, as in VANDAL-F, to signal the end of the absorber.

RHO may be set to zero for a void.

XTHICK may be set to zero to indicate a "spectrum sensor" at any point, including the front and back of the stack. In such a layer, BUCKL computes the currents and an estimate of the local energy spectrum. In this estimate, all diffuse (once-or-more-scattered) photons are assumed to have been degraded in energy by the average energy loss in a single Compton scattering. The error introduced by this assumption may be significant in thick absorbers. The front and back of a void are treated as spectrum sensors.

Both cards must be included for a sensor or a void, but the second may be blank. XTHICK, RHO, and NOZ may not be all zero. (Therefore, for a sensor, one must specify a fictitious RHO and/or NOZ.)

Adjacent voids and/or sensors will be combined and voids at either end of a stack converted to sensors. Any attempt to obtain information in the interior of a void (by making NSHELLS greater than 1) will be overruled. BUCKL automatically inserts a sensor at the back of the absorber.

8. A NEXTJOB card or deck in one of five forms to specify the next problem.

A. A card with FINISHED in Columns 1 to 8 ends the data deck. The program will then exit normally.

B. A card with SPEC/MAT in Columns 1 to 8 signals a completely new problem. It is followed by data elements 1 through 7 above.

C. A card with SPECTRUM in Columns 1 to 8, followed by data elements 1 through 4, will consider a new spectrum incident on the last-used material stack.

D. A card with MATERIAL in Columns 1 to 8, followed by data elements 3 through 7, will treat the last-used spectrum (perhaps renormalized to a new fluence) incident on a new material stack.

E. A card with FLUOR in Columns 1 to 5, followed by data elements 3, 4, and 5 will treat the last-used spectrum (perhaps renormalized to a new fluence) and last-used material stack with a new set of fluorescence lines.

Note that for a MATERIAL NEXTJOB, the last-used FLUOR flag is still in effect, and that a FLUOR NEXTJOB must contain a fluorescer deck.

Formats for input data and the arrangement of the data deck are shown on a schematic coding form in Fig. 15.

1	EMIN	8 9	DE	16 17	EMAX	24 25	DUMMY	32 33	PNCH	40 41	DUMMY	48 49	FLUOR	56 57	PRNT	64 65	PLOT	72 73	FATAL	80	
2	NAME																				
OR	B	10 11	W(1)	20 21	T(1)	30 31	W(2)	40 41	T(2)	50 51	W(3)	60 61	T(3)	70 71	W(4)	80					
OR	T(4)	8 9	16																		
2	S	FORMAT																			
OR	F(I)																				
OR	S ₁ / E ₁	8 9	16 17	24																	
2	E(I)																				
2	F(I)																				
3	FLUX																				
4	TITLE																				
5	NFL	4	5	14 15	24 25	34 35	44 45	54													
	IZ	EFL	K-YIELD	K-JUMP	L-YIELD	L-JUMP															
	IZ	EFL	K-YIELD	K-JUMP	L-YIELD	L-JUMP															
6	DIAM																				
7	XTHICK	8 9	RHO	16 17	NOZ	21 22	26	30 31	32 33	40 41	42 43	50 51	52 53	60 61	62 63	70 71	72 73	80			
	IZ	WT.FR	IZ	WT.FR	IZ	WT.FR	IZ	WT.FR	IZ	WT.FR	IZ	WT.FR	IZ	WT.FR	IZ	WT.FR	IZ	WT.FR			
	BLANK CARD																				
8	NEXTJOB																				

Fig. 15 Schematic coding form.

V. PROGRAM OUTPUT

The output from BUCKL is essentially similar to that from RANDAL⁴ which is, itself, a VANDAL descendant. Printed output includes a description of the absorber, including fluorescence parameters, spectral information, and a table of deposition results. The table contains, for each computational point, two VANDAL-type calculations, $(\rho^{-1}\sigma^{\text{abs}}_{\text{exp}}(-\sigma^{\text{abs}}_{\text{x}}))$ and $\rho^{-1}\sigma^{\text{abs}}_{\text{exp}}(-\sigma^{\text{tot}}_{\text{x}})$ (for comparison purposes only); BUCKL results, neglecting fluorescence (if any); the final BUCKL results in cal/gm and in megarads; and the ratio of final deposition to first interaction deposition (to indicate the relative importance of scattered buildup and/or fluorescence). For a spectrum sensor, the direct and reverse currents are given in cal/cm².

The plotted output contains the input spectrum; four deposition plots (the two VANDAL-type and BUCKL with and without fluorescence); spectral sensitivities $(d(\text{Deposition})/d(\text{Source Energy}))$ neglecting fluorescence) at the front and back of each material layer; and the estimates of the spectrum at each spectrum sensor. The spectral sensitivities and spectra are numbered sequentially from the source side of the absorber.

The punched output, if requested, consists of a title card, FORMAT (10A8), the transmitted current in cal/cm², FORMAT (E15.7), and the transmitted spectrum, including scattering and fluorescence and normalized to unit integral. The spectrum is punched with one energy (in keV) and intensity (in cal/cm²/keV) per card in FORMAT (2E15.7). Fluorescence lines have the arbitrary width DE, and it is assumed that trapezoid rule integrations will be used in interpreting the spectrum.

Since BUCKL will make some modifications to input data (e.g., supply EMAX and DE if missing, combine voids, or ignore fluorescers), it is imperative that the user check the program output to verify that input errors have not resulted in calculation of a problem different from that intended.

Appendix C is the Fortran listing for Program BUCKL.

VI. POSSIBLE FUTURE IMPROVEMENTS

One can think of several modifications which might be made to the BUCKL code in order to try to improve its accuracy, but we feel that these modifications would not produce sufficient improvement to justify the effort and the increased complexity of the code. We will, however, point out some of the accuracy-limiting approximations in BUCKL and suggest how the approximations might be improved should it become desirable at a later date.

1. The diffusion length $(3\sigma^{\text{abs}} \sigma^{\text{tr}})^{-1/2}$ is really only valid for scattering-dominated media. In the absorption-dominated limit it gives $3^{-1/2}(\sigma^{\text{abs}})^{-1}$ rather than the correct value of $(\sigma^{\text{abs}})^{-1}$. The correct formulation is well known,¹⁵ but the calculations required are rather involved. Since deposition by scattered radiation (D_2) vanishes in the absorption-dominated limit, the overall effects of this error are relatively small, except perhaps for fluorescence.

2. The fluorescence calculation could perhaps be improved by using an analytic first interaction deposition for fluorescence photons, expressible in terms of exponential integrals.

3. The Milne boundary condition at free surfaces is only an approximation because of distributed sources and, in any case, the extrapolation distance should really be a function of the ratio of scattering to absorption.¹⁵ The overall effect, however, is again small, as mentioned under item 1, above.

4. At a boundary between materials with greatly different values of $\sigma^{\text{abs}}/\sigma^{\text{tot}}$, the matching conditions used become inaccurate and could perhaps be improved. One way would be to include a transition region, as suggested by Ackroyd¹⁶ who outlines part of the necessary theory.

5. Empirical surface correction factors could be applied at interval free surfaces in finite radius problems containing voids.

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APPENDIX A
SAMPLE PROBLEM

APPENDIX A

SAMPLE PROBLEM

For a sample problem we will use the DTF test problem mentioned in the text.

A coding form with the data used is shown as Fig. A-1. We note several points about the data:

1. DE is set to 20.0, although the source spectrum is zero below 25.88 so that fluorescence lines will appear on plots at their correct energies.
2. The segmented spectrum option (S/E) is used and the spectrum normalized to 1.0 to give a normalized deposition.
3. The terms f_K and ω^K have been specified so that their product has the value used in the DTF report; the value of $E_{F\ell}$ is also from that report. Ordinarily, one would specify only the Z numbers and use BUCKL's fits for the other fluorescence parameter.
4. A large diameter has been used to give slab geometry.
5. A void, which BUCKL will convert to a spectrum sensor has been placed in front of the absorber to evaluate the "reflected" current which will consist primarily of fluorescence photons in this case.
6. A completely unrelated job will be run next.

The printed output for this problem is shown in Figs. A-2 and A-3. Here the columns headed AB, AB and AB, TOT are the exponential results $\rho^{-1}\sigma^{abs} \exp(-\sigma^{abs}x)$ and $\rho^{-1}\sigma^{abs} \exp(-\sigma^{tot}x)$, respectively. The first is essentially VANDAL, and the second, the first-interaction deposition. NO FLUOR, is the BUCKL result before consideration of fluorescence. All are in cal/gm. DEP (CAL/GM) and DEP(MR) are the final BUCKL result in two sets of units, and DEP/A,T is the ratio of total deposition to deposition at first interaction, the "buildup factor."

Date _____
Program _____

FOR COMMENT COLUMN		NOTATION		FORTRAN STATEMENT	
STATEMENT NUMBER		B = blank 0 = Zero	D = 0 (letter) 1 = 1 (one)	I = i (letter) X = x (letter) 2 = two	
1	2	3	4	5	6
20.0	0.1	40.0			
S/E	(10F8.0)	4			
0.0	25.87	25.88	50.0		
0.0	0.0	25.88	50.0		
1.0					
TEST	PROBLEM FROM DTF REPORT - NORMALIZED				
4					
47	22.40	0.830	0.7771		
50	25.78	0.860	0.7802		
51	26.80	0.866	0.7841		
52	28.03	0.872	0.7959		
999999	999.				
1.					
BLANK					
.006	5.76	3	10		
47 32 3	.61 51 121.75	16	96.96		
.008	1.96	1	10		
16 1.0					
.006	6.48	12	10		
50 1 13	.69 152.127.60				
BLANK					
SPEC/MAT					
FINISHED					

Fig. A-1 Data for DTF test problem.

BUCKL CALCULATION
 S/E SPECTRUM EMIN= 20.0000 DE= .1000 EMAX= 40.0000

CURRENT = 1.00000 CAL/SQCM

LAYER	THICKNESS	DIAH(CM)	DENSITY	Z	WT.FR.	Z	WT.FR.	Z	WT.FR.	Z	WT.FR.	Z	WT.FR.	Z	WT.FR.
1	0.000000*99999.000														
2	.006000*99999.000		5.760	47	.5976	51	.2248	16	.1776						
3	.008000*99999.000		1.960	16	1.0000										
4	.006000*99999.000		6.480	50	.4819	52	.5181								
5	0.000000*99999.000														

THESE ELEMENTS ALLOWED TO FLUORESC

Z	FL.ENERGY	YIELD	K-JUMP	L-JUMP
52	28.0300	.8720	.7959	
51	26.8000	.8660	.7841	
50	25.7800	.8600	.7802	
47	22.4000	.8300	.7771	

TEST PROBLEM FROM DTF REPORT

Fig. A-2 Printed output for DTF test problem.

TEST PROBLEM FROM DTF REPORT

INCIDENT FLUX = 1.00E+00

X(CM)	AB,AB	AB,TOT	NO FLUOR	DEP/A,T	DEP(CAL/GM)	DEP(MR)	+CURRENT	-CURRENT
0.00000							1.000E+00	1.066E-01
0.00000	2.415E+01	2.415E+01	2.419E+01	.666	1.608E+01	6.720E+00		
.00060	2.212E+01	2.211E+01	2.217E+01	.701	1.551E+01	6.483E+00		
.00120	2.028E+01	2.026E+01	2.033E+01	.731	1.480E+01	6.186E+00		
.00180	1.859E+01	1.857E+01	1.864E+01	.758	1.408E+01	5.884E+00		
.00240	1.705E+01	1.702E+01	1.710E+01	.787	1.339E+01	5.597E+00		
.00300	1.565E+01	1.561E+01	1.569E+01	.818	1.277E+01	5.336E+00		
.00360	1.436E+01	1.432E+01	1.440E+01	.853	1.221E+01	5.105E+00		
.00420	1.319E+01	1.314E+01	1.322E+01	.893	1.174E+01	4.906E+00		
.00480	1.211E+01	1.206E+01	1.215E+01	.941	1.135E+01	4.743E+00		
.00540	1.113E+01	1.108E+01	1.116E+01	.997	1.104E+01	4.617E+00		
.00600	1.023E+01	1.018E+01	1.026E+01	1.065	1.083E+01	4.528E+00		

.00600	5.717E-01	5.687E-01	5.743E-01	3.288	1.870E+00	7.817E-01		
.00680	5.703E-01	5.672E-01	5.728E-01	3.276	1.858E+00	7.768E-01		
.00760	5.690E-01	5.657E-01	5.713E-01	3.265	1.847E+00	7.720E-01		
.00840	5.676E-01	5.643E-01	5.698E-01	3.253	1.836E+00	7.673E-01		
.00920	5.663E-01	5.628E-01	5.683E-01	3.242	1.824E+00	7.626E-01		
.01000	5.650E-01	5.613E-01	5.668E-01	3.230	1.813E+00	7.579E-01		
.01080	5.636E-01	5.598E-01	5.654E-01	3.219	1.802E+00	7.533E-01		
.01160	5.623E-01	5.584E-01	5.639E-01	3.208	1.791E+00	7.488E-01		
.01240	5.610E-01	5.569E-01	5.624E-01	3.197	1.781E+00	7.443E-01		
.01320	5.597E-01	5.555E-01	5.610E-01	3.187	1.770E+00	7.399E-01		
.01400	5.583E-01	5.540E-01	5.595E-01	3.176	1.760E+00	7.355E-01		

.01400	1.043E+01	1.035E+01	1.043E+01	.991	1.026E+01	4.288E+00		
.01460	9.412E+00	9.334E+00	9.406E+00	1.004	9.372E+00	3.918E+00		
.01520	8.500E+00	8.426E+00	8.491E+00	1.018	8.574E+00	3.584E+00		
.01580	7.682E+00	7.611E+00	7.669E+00	1.032	7.855E+00	3.283E+00		
.01640	6.947E+00	6.879E+00	6.932E+00	1.047	7.204E+00	3.011E+00		
.01700	6.287E+00	6.222E+00	6.269E+00	1.063	6.613E+00	2.764E+00		
.01760	5.693E+00	5.631E+00	5.674E+00	1.078	6.072E+00	2.538E+00		
.01820	5.159E+00	5.100E+00	5.138E+00	1.092	5.571E+00	2.329E+00		
.01880	4.678E+00	4.622E+00	4.655E+00	1.103	5.100E+00	2.132E+00		
.01940	4.245E+00	4.192E+00	4.220E+00	1.108	4.645E+00	1.942E+00		
.02000	3.854E+00	3.804E+00	3.827E+00	1.102	4.191E+00	1.752E+00		
.02000							2.574E-01	0.

Fig. A-3 Printed output for DTF test problem.

APPENDIX B

DIMENSION LIMITS

APPENDIX B

DIMENSION LIMITS

The arrays in BUCKL are dimensioned to permit problems with the following dimension limits:

NE=number of photon energies ≤ 400 (e)

NL=number of layers including sensors and voids ≤ 20 (l)

MATM=number of material layers ≤ 10 (m)

NSP=number of calculational points ≤ 400 (p)

(Note that a layer with NSHELLS=10 contains 11 points)

ISPEC=number of sensors ≤ 10 (s)

NOZ=number of elements in a layer ≤ 10 (z)

NZF=number of fluorescence lines ≤ 10 (f)

To increase these limits one must change dimension statements as follows (letters refer to the maximum values of the variables in BUCKL above):

```
DIMENSION ELEVEL(e),NFL(m,z),FRB(m,f),FRD(m,f),IZF(f),
1 DPA(p),DPT(p),DP1(p),DP3(p),DP(p),SPSS(e,m),
2 SPSB(e,m),XT(l),LS(l),XP(p),LOZ(l),NZZ(m,z),W(m,z),
3 RHOO(m),SABS(m),SABSD(m),STRD(m),MAT(m),SPEC(e,s),
4 FLSOUR(p,f),CON(f),CIN(f),IZZ(f),EFL(f),IV(4),NJ(5),LN(7)
```

in SQUID

```
DIMENSION OM(2m),BET(2m),GAM(2m),DEL(2m)
```

IN PLOUT

```
DIMENSION X(max(e,p)),Y(max(e,p),max(m,s)),LAB(10)
```

COMMON blocks must also be changed, noting any name changes in subroutines

```
COMMON/SPECT/EMIN,DE,EMAX,NE,FLEVEL(e),E(e)
COMMON/FLUOR/NZFL,IZFL(f),EKE(f),ELE(f)
COMMON/EVALU/F(2m),B(2m),C(2m),D(2m),H(2m),V(2m),G(2m),M2
COMMON/COEFF/AK(m),DELT(m),STTL(m),A(m),EXK(m),EXS(m),MATM,
1 XSKIP(m),YYZ
```

One must also change array initializations or dimension checks on the following cards: BKL51, BKL57, BKL60, BKL65, BKL92, BKL135, BKL192-193, BKL199-208, and BKL224-226.

APPENDIX C

FORTRAN LISTING

APPENDIX C

FORTTRAN LISTING

```

PROGRAM BUCKL(INPUT,OUTPUT,PUNCH,TAPE15,TAPE40)      BKL 1
C THIS IS A FAST ANALYTIC DEPOSITION CODE INCORPORATING A BUCKLING      BKL 2
C CORRECTION FOR FINITE TRANSVERSE GEOMETRY. 400 ENERGY POINTS,      BKL 3
C 10 LAYERS, 400 COMPUTATIONAL POINTS, 10 FLUORESCERS      BKL 4
COMMON/SPECT/EMIN,DE,EMAX,NE,FLEVEL(400),E(400)      BKL 5
COMMON/TITLE/VIC(10)      BKL 6
COMMON/BIGG/IZ,EARG,PH,AB,TOT      BKL 7
COMMON/FLUOR/NZFL,IZFL(10),EKE(10),ELE(10)      BKL 8
COMMON/EVALU/F(20),B(20),C(20),D(20),H(20),V(20),G(20),M2      BKL 9
COMMON/COEFF/A<(10),DELTA(10),STTL(10),A(10),EXK(10),EXS(10),MATM,      BKL 10
1 XSKIP(10),YYZ      BKL 11
DIMENSION FLEVEL(400),NFL(10,10),FRB(10,10),FRD(10,10),IZF(10),      BKL 12
1 DPA(400),DPT(400),DP1(400),DP3(400),DP(400),SPSS(400,10),      BKL 13
2 SPSB(400,10),XT(20),LS(20),XP(400),LOZ(20),NZZ(10,10),W(10,10),      BKL 14
3 RHOO(10),SABS(10),SABSD(10),STRD(10),MAT(10),SPEC(400,10),      BKL 15
4 FLSOUR(400,10),CON(10),CIN(10),IZZ(10),EFL(10),IV(4),NJ(5),LN(7)      BKL 16
DATA (LN=4H NE,4H NZF,4H NL,4H NOZ,4HMATM,4HSPEC,4H NSP)      BKL 17
DATA (NJ=8HFINISHED,8HSPEC/MAT,8HSPECTRUM,8HMATERIAL,8HFLUOR),      BKL 18
1 (IV=8HSPECTRUM,7H SENSOR,4HVOID,1H ),(ISTAR=8H*****))      BKL 19
SCATRAT(E)=2.35E-3*LE/(1.+2.98257E-3*EE*(1.+1.62736E-5*EE*(1.-2.18E-2      BKL 20
14922E-2*FF)))      BKL 21
SURL(X)=1.-0.28*EXP(-10.*X)      BKL 22
SURL(X)=1.-0.18*EXP(-7.3*X)      BKL 23
FLEK(X)=(6.7527E-3+X*(7.5653E-6+X*(-1.72567E-7+X*2.0019E-9)))*X**2      BKL 24
1.104      BKL 25
FLEL(X)=(1.35427E-4+X*(-1.13774E-7+X*(-8.8858E-9+X*6.2853E-11)))*X      BKL 26
1**2.6458      BKL 27
RATK(X)=0.957-X*(2.51E-3-6.0E-6*X)      BKL 28
RATL(X)=1.000-X*(4.42E-3-1.967E-5*X)      BKL 29
FEFFK(X)=(.9463+(18.045/X)**2)/(1.0+(35.374/X)**4)      BKL 30
FEFFL(X)=AMAX1(.00621*X-.199,1./(2.08+(75.5/X)**10))      BKL 31
CALL BIGGR      BKL 32
ISKIP=0      BKL 33
C DEFINE SPECTRAL POINTS AND OBTAIN NORMALIZED SPECTRUM      BKL 34
10 READ 850, EMIN,DE,EMAX,PUNCH,FLUOR,PRNT,PLOTT,FATAL      BKL 35
PRINT 840      BKL 36
IF (DE.LE.0.) DE=0.1      BKL 37
IF ((EMAX-EMIN).GT.398.*DE) DE=(EMAX-EMIN)/398.      BKL 38
IF (EMAX.LT.EMIN) EMAX=EMIN      BKL 39
NE=(EMAX-EMIN)/DE+1.1      BKL 40
DO 20 I=1,NE      BKL 41
20 E(I)=EMIN+DE*(I-1)      BKL 42
CALL INTENS (IERR)      BKL 43
IF (IERR.NE.0) GO TO 780      BKL 44
C READ FLUENCE AND RENORMALIZE SPECTRUM      BKL 45
30 READ 850, CVR      BKL 46
DO 40 I=1,NE      BKL 47
40 ELEVEL(I)=FLEVEL(I)*CVR      BKL 48
PRINT 880, CVB      BKL 49
READ 940, (VIC(I),I=1,10)      BKL 50
IF (NE.LE.400) GO TO 50      BKL 51
PRINT 860, (VIC(LL),LL=1,10),LN(1),NE      BKL 52
GO TO 780      BKL 53
C PLOT INCIDENT SPECTRUM      BKL 54

```

50	IF (PLOTT.EQ.0.) CALL PLOUT (E,ELEVEL,NE,6,1,1)	BKL	55
	IF (ISKIP) 80,61,350	BKL	56
60	DO 7 I=1,1	BKL	57
70	NZZ(I)=0	BKL	58
80	DO 9 I=1,1	BKL	59
90	NFL(I)=1	BKL	60
	NZFL=0	BKL	61
	NZF=0	BKL	62
	IF (FLUOR.EQ.0..AND.ISKIP.EQ.0) GO TO 110	BKL	63
	READ 870, NZF	BKL	64
	IF (NZF.LE.1) GO TO 100	BKL	65
	PRINT 860, (VIC(LL),LL=1,10),LN(2),NZF	BKL	66
	GO TO 780	BKL	67
100	READ 870, (IZFL(I),A(I),F(I),B(I),C(I),D(I),I=1,NZF)	BKL	68
	IF (ISKIP.LT.0) GO TO 240	BKL	69
110	PRINT 890	BKL	70
C	READ DIAMETER OF STACK	BKL	71
	READ 1010, YYZ	BKL	72
	NL=0	BKL	73
	MATM=0	BKL	74
	ISPEC=0	BKL	75
C	READ DEFINITION OF NEXT HOMOGENOUS LAYER	BKL	76
120	READ 900, XTHICK,RHO,NOZ,NSHELLS	BKL	77
	IF (XTHICK.LE.0..AND.RHO.LE.0..AND.NOZ.LE.0) GO TO 170	BKL	78
	NL=NL+1	BKL	79
	IF (XTHICK.LT.0.) XTHICK=0.0	BKL	80
C	NEXT CARD SETS MINIMUM DENSITY FOR A REAL MATERIAL	BKL	81
	IF (RHO.LT.1.E-4) RHO=0.	BKL	82
	IF (XTHICK*RHO.GT.0.) GO TO 130	BKL	83
	READ 940, IDUM	BKL	84
	XT(NL)=0.	BKL	85
	LOZ(NL)=0	BKL	86
	IF (NL.EQ.1) GO TO 120	BKL	87
	IF (LOZ(NL-1).EQ.0) NL=NL-1	BKL	88
	XT(NL)=XT(NL)+XTHICK*AMINO(1,NL-1)	BKL	89
	GO TO 120	BKL	90
130	XT(NL)=XTHICK	BKL	91
	IF (NOZ.LE.10) GO TO 140	BKL	92
	PRINT 860, (VIC(LL),LL=1,10),LN(3),NL,LN(4),NOZ	BKL	93
	GO TO 780	BKL	94
140	MATM=MATM+1	BKL	95
	RHO0(MATM)=RHO	BKL	96
	READ 910, (NZZ(MATM,I),A(MATM,I),I=1,NOZ)	BKL	97
	LOZ(NL)=NOZ	BKL	98
	LS(NL)=NSHELLS+1	BKL	99
	SUM=0.0	BKL	100
C	NORMALIZE ELEMENTAL WEIGHT FRACTIONS	BKL	101
	DO 150 I=1,NOZ	BKL	102
150	SUM=SUM+W(MATM,I)	BKL	103
	DO 160 I=1,NOZ	BKL	104
160	W(MATM,I)=W(MATM,I)/SUM	BKL	105
	GO TO 120	BKL	106
170	IF (LOZ(NL).EQ.0) GO TO 180	BKL	107
	NL=NL+1	BKL	108

18	LOZ(NL)=	BKL	109
	XT(NL)=0.0	BKL	110
	KL=NL	BKL	111
	XTP=0.0	BKL	112
	NSP=0	BKL	113
	M=0	BKL	114
	DO 220 KK=1,NL	BKL	115
	IF (LOZ(KK).GT.0) GO TO 190	BKL	116
	IF (XT(KK).GT.0) LOZ(KK)=-1	BKL	117
	NSHELLS=-LOZ(KK)	BKL	118
	PRINT 930, KK,XT(KK),YYZ,IV(2*NSHELLS+1),IV(2*NSHELLS+2)	BKL	119
	LS(KK)=NSHELLS+1	BKL	120
	ISPEC=ISPEC+LS(KK)	BKL	121
	GO TO 200	BKL	122
190	NSHELLS=LS(KK)-1	BKL	123
	NOZ=LOZ(KK)	BKL	124
	M=M+1	BKL	125
	MAT(M)=KK	BKL	126
	XSKIP(M)=0.0	BKL	127
	IF (LOZ(KK+1).LT.0) XSKIP(M)=XT(KK+1)	BKL	128
	PRINT 92, KK,XT(KK),YYZ,RHOO(M),(NZZ(M,J),W(M,J),J=1,NOZ)	BKL	129
200	NS=NSHELLS+1	BKL	130
	DX=0.0	BKL	131
	IF (NSHELLS.GT.0) DX=XT(KK)/FLOAT(NSHELLS)	BKL	132
	DO 210 I=1,NS	BKL	133
	II=NSP+I	BKL	134
	IF (II.GT.400) GO TO 220	BKL	135
210	XP(II)=XTP+DX*(I-1)	BKL	136
220	NSP=NSP+NS	BKL	137
230	XTP=XTP+XT(KK)	BKL	138
	IF (NZF.LE.0) GO TO 350	BKL	139
C	REORDER FLUORESCERS BY DECREASING FLUORESCENCE ENERGY	BKL	140
240	PRINT 990	BKL	141
	DO 270 N=1,NZF	BKL	142
	IF (A(N).GT.0.) GO TO 270	BKL	143
	IF (IZFL(N)) 250,270,260	BKL	144
250	A(N)=FLEL(FLOAT(-IZFL(N)))	BKL	145
	GO TO 270	BKL	146
260	A(N)=FLEK(FLOAT(IZFL(N)))	BKL	147
270	CONTINUE	BKL	148
	DO 290 N=1,NZF	BKL	149
	EE=0.0	BKL	150
	DO 280 I=1,NZF	BKL	151
	IF (A(I).LT.FE) GO TO 280	BKL	152
	EE=A(I)	BKL	153
	ISAVE=I	BKL	154
280	CONTINUE	BKL	155
	IZF(N)=IZFL(ISAVE)	BKL	156
	IZZ(N)=ISAVE	BKL	157
290	A(ISAVE)=-A(ISAVE)	BKL	158
	DO 340 J=1,NZF	BKL	159
	IF (IZF(J).LT.15.AND.IZF(J).GT.-40) GO TO 340	BKL	160
	IKEY=0	BKL	161
	IF (J.EQ.1) GO TO 300	BKL	162

300	IF (IZF(J)-IZF(J-1)) 300,340,300	BKL	163
	DO 340 K=1,MATM	BKL	164
	M=MAT(K)	BKL	165
	NQZ=LOZ(M)	BKL	166
	DO 340 I=1,NQZ	BKL	167
	IF (NZZ(K,I).NE.IARS(IZF(J))) GO TO 340	BKL	168
	IF (IKEY.EQ.1) GO TO 330	BKL	169
	IKEY=1	BKL	170
	NZFL=NZFL+1	BKL	171
	ISAVE=IZZ(J)	BKL	172
	FFL(NZFL)=-A(ISAVE)	BKL	173
	Z=IARS(IZF(J))	BKL	174
	IF (B(ISAVE).LE.0.) B(ISAVE)=RATK(Z)	BKL	175
	IF (IZF(J).GT.0) GO TO 31	BKL	176
	IF (C(ISAVE).LL.0.) C(ISAVE)=FEFFL(Z)	BKL	177
	IF (D(ISAVE).LE.0.) D(ISAVE)=RATL(Z)	BKL	178
	CON(NZFL)=C(ISAVE)*D(ISAVE)*EFL(NZFL)	BKL	179
	CIN(NZFL)=1.-B(ISAVE)	BKL	180
	PRINT 870, IZF(J),EFL(NZFL),C(ISAVE),B(ISAVE),D(ISAVE)	BKL	181
	NADD=1000*NZFL	BKL	182
	GO TO 320	BKL	183
310	IF (F(ISAVE).EQ.0.) F(ISAVE)=FEFFK(Z)	BKL	184
	CON(NZFL)=F(ISAVE)*B(ISAVE)*EFL(NZFL)	BKL	185
	PRINT 870, IZF(J),EFL(NZFL),F(ISAVE),B(ISAVE)	BKL	186
	NADD=NZFL	BKL	187
320	IZFL(NZFL)=IZF(J)	BKL	188
330	NFL(K,I)=NFL(K,I)+NADD	BKL	189
340	CONTINUE	BKL	190
	CALL BIGGSF	BKL	191
350	IF (NL.LE.20.AND.MATM.LE.10.AND.ISPEC.LE.10.AND.NSP.LE.400) GO TO 1360	BKL	192
	PRINT 860, (VIC(LL),LL=1,10),LN(3),NL,LN(5),MATM,LN(6),ISPEC,LN(7)	BKL	193
	1,NSP	BKL	194
	GO TO 780	BKL	195
360	PRINT 1000, (VIC(LL),LL=1,10)	BKL	196
C	SET ALL F SUMS TO ZERO	BKL	197
	DO 370 J=1,400	BKL	198
	DPA(J)=0.0	BKL	199
	DPT(J)=0.0	BKL	200
	DP3(J)=0.0	BKL	201
370	DP(J)=0.0	BKL	202
	DO 380 J=1,4000	BKL	203
	FLSOUR(J)=0.0	BKL	204
	SPSS(J)=0.0	BKL	205
	SPSR(J)=0.0	BKL	206
380	SPEC(J)=0.0	BKL	207
	M2=7*MATM	BKL	208
	IDONE=0	BKL	209
C	ENERGY LOOP	BKL	210
	DO 510 I=1,NE	BKL	211
	IF (ELEVEL(I).EQ.0.) GO TO 510	BKL	212
	CIC=1.0	BKL	213
	IF (I.EQ.1.OR.I.EQ.NE) CIC=.5	BKL	214
	EF=E(I)	BKL	215
		BKL	216

EDEG=EE*(1.+2.6258E-3*EE)/(1.+4.5533E-3*EE*(1.+2.0454E-4*EE))	BKL	217
IDEG=(EDEG-EMIN)/DE+1.1	BKL	218
IF (IDEG.LT.1) IDEG=1	BKL	219
FRR=(EDEG-E(IDEG))/DE	BKL	220
IF (FRR.LT.0.) FRR=0.0	BKL	221
300 AT=1.0	BKL	222
TAUS=).	BKL	223
DO 400 L=1,100	BKL	224
FRR(L)=0.0	BKL	225
400 FRD(L)=0.0	BKL	226
C CALCULATE ALL CONSTANTS FOR EACH LAYER	BKL	227
DO 460 J=1,MATM	BKL	228
M=MAT(J)	BKL	229
MOZ=LOZ(M)	BKL	230
STOT=0.0	BKL	231
SAR=0.0	BKL	232
SARD=0.0	BKL	233
STOTD=0.0	BKL	234
DO 420 K=1,MOZ	BKL	235
IZ=NZZ(J,K)	BKL	236
WW=RHOO(J)*W(J,K)	BKL	237
EARG=EE	BKL	238
CALL RIGGS	BKL	239
SAR=SAR+AR*WW	BKL	240
STOT=STOT+TOT*WW	BKL	241
PE=PH	BKL	242
EARG=EDEG	BKL	243
CALL RIGGS	BKL	244
SARD=SARD+AR*WW	BKL	245
PD=PH	BKL	246
N=NFL(J,K)/1000	BKL	247
IF (N.EQ.0) GO TO 410	BKL	248
IF (EE.GT.EKE(N)) FRB(J,N)=PE*WW	BKL	249
IF (EE.GT.EKE(N)) FRB(J,N)=FRB(J,N)*CIN(N)	BKL	250
IF (EDEG.GT.ELE(N)) FRD(J,N)=PD*WW	BKL	251
IF (EDEG.GT.EKE(N)) FRD(J,N)=FRD(J,N)*CIN(N)	BKL	252
410 N=MOD(NFL(J,K),1000)	BKL	253
IF (N.EQ.0) GO TO 420	BKL	254
IF (EE.GT.EKE(N)) FRB(J,N)=PE*WW	BKL	255
IF (EDEG.GT.EKE(N)) FRD(J,N)=PD*WW	BKL	256
420 STOTD=STOTD+TOT*WW	BKL	257
SARS(J)=SAR	BKL	258
STTL(J)=STOT	BKL	259
SABSD(J)=SARD	BKL	260
IF (NZFL.EQ.0) GO TO 440	BKL	261
DO 430 N=1,NZFL	BKL	262
IF (FRB(J,N).EQ.0.) GO TO 430	BKL	263
FRB(J,N)=FRB(J,N)*CON(N)/(EE*SARS(J))	BKL	264
IF (FRD(J,N).EQ.0.) GO TO 430	BKL	265
FRD(J,N)=FRD(J,N)*CON(N)/(EDEG*SABSD(J))	BKL	266
430 CONTINUE	BKL	267
440 CONTINUE	BKL	268
STR=STOTD-(STOTD-SABSD(J))*SCATRAT(EDEG)	BKL	269
STRD(J)=STR	BKL	270

	DFLT(J)=.71/STR	BKL	271
	RSTAR=.5*YYZ+(J.71-0.49*EXP(-2.5*YYZ*STR)-0.21)*EXP(-20.*YYZ*STR)	BKL	272
	1)/STR	BKL	273
	BK=3.*SABSD(J)*STR+5.784/(RSTAR*RSTAR)	BKL	274
	A(J)=J.0	BKL	275
	IF (IDONE.NE.) GO TO 45	BKL	276
	STOT2=STTL(J)*STTL(J)	BKL	277
	DIFF=BK-STOT2	BKL	278
	IF (ABS(DIFF).LT.1.E-4*STOT2) BK=BK*(1.0+SIGN(1.E-4,DIFF))	BKL	279
	A(J)=AT*3.*(STTL(J)-SABS(J))*(STR+STTL(J)*SCATNAT(LE))/(BK-STOT2)	BKL	280
450	AK(J)=SQRT(BK)	BKL	281
	EXS(J)=EXP(-STTL(J)*XT(M))	BKL	282
	AT=AT*FXS(J)	BKL	283
	TAUS=TAUS+XT(M)*STR	BKL	284
	EXK(J)=EXP(-AK(J)*XT(M))	BKL	285
460	CONTINUE	BKL	286
C	CALCULATE COEFFICIENTS	BKL	287
	CALL COEF	BKL	288
	IF (IDONE.EQ.1) GO TO 520	BKL	289
	CALL SQUID	BKL	290
C	CALCULATE DEPOSITION AT EACH POINT	BKL	291
	AT=1.0	BKL	292
	AA=1.0	BKL	293
	MSP=0	BKL	294
	TAU=J.0	BKL	295
	J=1	BKL	296
	ISPEC=J	BKL	297
	DO 500 M=1,MATM	BKL	298
	SAB=SABS(M)	BKL	299
	STOT=STTL(M)	BKL	300
	AKK=AK(M)	BKL	301
	STR=STRD(M)	BKL	302
	AR=CIC*FLEVEL(I)/RHOO(M)	BKL	303
	ARC=AR*SAB	BKL	304
	ARCA=ARC*AA	BKL	305
	ARCT=ARC*AT	BKL	306
	ARCD=AR*SABSD(M)	BKL	307
	AAZ=A(M)	BKL	308
	BBZ=V(2*M-1)	BKL	309
	CCZ=V(2*M)	BKL	310
	EXX=EXK(M)	BKL	311
	IF (J.EQ.MAT(M)) GO TO 470	BKL	312
	MSP=MSP+1	BKL	313
	SF=SURL(TAU)*SURR(TAUS-TAU)	BKL	314
	DDP=ELEVEL(I)*(AAZ+BBZ+CCZ*EXX)*SF	BKL	315
	DDP1=ELEVEL(I)*(-AAZ*STOT+(CCZ*EXX-BBZ)*AKK)*SF	BKL	316
	DDP2=ELEVEL(I)*AT	BKL	317
	DP(MSP)=DP(MSP)+CIC*(0.25*(DDP-DELTA(M)*DDP1)+DDP2)	BKL	318
	DP3(MSP)=DP3(MSP)+CIC*0.25*(DDP+DELTA(M)*DDP1)	BKL	319
	ISPEC=ISPEC+1	BKL	320
	SPEC(I,ISPEC)=SPEC(I,ISPEC)+DDP2	BKL	321
	SPEC(IDEG,ISPEC)=SPEC(IDEG,ISPEC)+(1.-FRR)*DDP	BKL	322
	SPEC(IDEG+1,ISPEC)=SPEC(IDEG+1,ISPEC)+FRR*DDP	BKL	323
	J=J+1	BKL	324

470	KK=LS(J)	BKL	325
	Z7L=XP(MSP+1)	BKL	326
	XTK=XT(J)	BKL	327
	DO 490 K=1, KK	BKL	328
	MTOT=MSP+K	BKL	329
	ZZ=XP(MTOT)-ZZL	BKL	330
	TAUT=TAU+ZZ*STR	BKL	331
	EXAZ=EXP(-SAR*ZZ)	BKL	332
	EXSZ=EXP(-STOT*ZZ)	BKL	333
	EXKZ=EXP(-AKK*ZZ)	BKL	334
	FXXP=EXP(AKK*(ZZ-XTK))	BKL	335
	DDP1=ABCT*EXSZ	BKL	336
	DDP=ABCD*(AAZ*EXSZ+BBZ*EXKZ+CCZ*EXKR)*SURL(TAUT)*SURR(TAUT-TAUT)+DBKL	BKL	337
	DDP1	BKL	338
	DPA(MTOT)=DPA(MTOT)+ABCA*EXAZ	BKL	339
	DPT(MTOT)=DPT(MTOT)+DDP1	BKL	340
	DP3(MTOT)=DP3(MTOT)+DDP	BKL	341
C	CALCULATE SPECTRAL SENSITIVITY AT LAYER FRONT AND BACK	BKL	342
	IF (K.EQ.1) SPSS(I,M)=DDP/CIC	BKL	343
	IF (K.EQ.KK) SPSB(I,M)=DDP/CIC	BKL	344
	IF (NZFL.FQ.0) GO TO 490	BKL	345
	DO 480 N=1, NZFL	BKL	346
	DPF=DDP1*FRB(M,N)+(DDP-DDP1)*FRD(M,N)	BKL	347
	FLSOUR(MTOT,N)=FLSOUR(MTOT,N)+DPF	BKL	348
480	DP(MTOT)=DP(MTOT)-DPF	BKL	349
490	DP(MTOT)=DP(MTOT)+DDP	BKL	350
	AA=AA*FXA7	BKL	351
	AT=AT*FXSZ	BKL	352
	TAU=TAU+XT(J)*STR	BKL	353
	MSP=MSP+LS(J)	BKL	354
	J=J+1	BKL	355
	IF (LOZ(J).GT.0) GO TO 500	BKL	356
	MSP=MSP+1	BKL	357
	SF=SURL(TAU)*SURR(TAUT-TAU)	BKL	358
	DDP=ELEVEL(I)*(AAZ*EXSZ+BBZ*EXX+CCZ)*SF	BKL	359
	DDP1=ELEVEL(I)*(-STOT*AAZ*EXSZ+AKK*(CCZ-BBZ*EXX))*SF	BKL	360
	DDP2=ELEVFL(I)*AT	BKL	361
	DP(MSP)=DP(MSP)+CIC*(0.25*(DDP-DELT(M)*DDP1)+DDP2)	BKL	362
	DP3(MSP)=DP3(MSP)+CIC*0.25*(DDP+DELT(M)*DDP1)	BKL	363
	ISPFC=ISPFC+1	BKL	364
	SPEC(I,ISPFC)=SPEC(I,ISPFC)+DDP2	BKL	365
	SPEC(IDEG,ISPFC)=SPEC(IDEG,ISPFC)+(1.-FRR)*DDP	BKL	366
	SPEC(IDEG+1,ISPFC)=SPEC(IDEG+1,ISPFC)+FRR*DDP	BKL	367
500	IF (LOZ(J).EQ.0) J=J+1	BKL	368
510	CONTINUE	BKL	369
	IDONE=1	BKL	370
	IF (NZFL.EQ.0) GO TO 680	BKL	371
	DO 670 NF=1, NZFL	BKL	372
	NF1=NF+1	BKL	373
	FF=FFL(NF)	BKL	374
	EDEG=FE	BKL	375
	I=(EE-EMIN)/DE+1.	BKL	376
	IF (I.LT.1) I=1	BKL	377
	GO TO 390	BKL	378

520	DO 530 J=1,NSP	BKL	379
530	DP1(J)=0.0	BKL	380
	MSP=1	BKL	381
	J=1	BKL	382
	DO 600 M=1,MATM	BKL	383
	IF (J.EQ.MAT(M)) GO TO 540	BKL	384
	MSP=MSP+LS(J)	BKL	385
	J=J+1	BKL	386
540	NI=LS(J)-1	BKL	387
	IF (FLSOUR(MSP,NF).EQ.0.) GO TO 590	BKL	388
	AKK=AK(M)	BKL	389
	C0=1.5*RHO0(M)*STRD(M)/AKK	BKL	390
	XL=XP(MSP)	BKL	391
	DO 580 II=1,NI	BKL	392
	MSRC=MSP+II-1	BKL	393
	XR=XP(MSRC+1)	BKL	394
	DX=XR-XL	BKL	395
	FXX=FXP(-AKK*DX)	BKL	396
	RAT=FLSOUR(MSRC+1,NF)/FLSOUR(MSRC,NF)	BKL	397
	GAM=-ALOG(RAT)/DX	BKL	398
	DIFF=AKK-ARS(GAM)	BKL	399
	IF (ABS(DIFF).GT.1.E-6*GAM) GO TO 550	BKL	400
	GAM=GAM*(1.0-SIGN(1.E-6,DIFF))	BKL	401
	RAT=FXP(-GAM*DX)	BKL	402
550	C1=C0*FLSOUR(MSRC,NF)	BKL	403
	C2=C1*(1.-RAT*EXX)/(AKK+GAM)	BKL	404
	C1=C1*(RAT-EXX)/(AKK-GAM)	BKL	405
	DO 560 L=1,II	BKL	406
	MPT=MSRC+1-L	BKL	407
560	DP1(MPT)=DP1(MPT)+C2*EXP(AKK*(XP(MPT)-XL))	BKL	408
	LAST=LS(J)-II	BKL	409
	DO 570 L=1,LAST	BKL	410
	MPT=MSRC+L	BKL	411
570	DP1(MPT)=DP1(MPT)+C1*EXP(AKK*(XR-XP(MPT)))	BKL	412
580	XL=XR	BKL	413
590	V(2*M-1)=DP1(MSP)	BKL	414
	V(2*M)=DP1(MSP+NI)	BKL	415
	MSP=MSP+LS(J)	BKL	416
600	J=J+1	BKL	417
C	EVALUATE CONSTANT ARRAY	BKL	418
	G(1)=V(1)*(1.-AK(1)*DELT(1))	BKL	419
	IF (MATM.EQ.1) GO TO 620	BKL	420
	MM1=MATM-1	BKL	421
	DO 610 L=1,MM1	BKL	422
	LR=L+1	BKL	423
	X=XSKIP(L)*2./YYZ	BKL	424
	F1=(1.+0.2271*X)/(1.+1.7672*X*(1.+0.7621*X*(1.+0.2792*X)))	BKL	425
	F2=(1.+0.13182*X)/(1.+0.5930*X*(1.+0.9550*X*(1.+0.15551*X)))	BKL	426
	G(2*L)=-V(2*L)*(1.-AK(L)*DELT(L))+V(2*L+1)*(F1+F2*AK(LR)*DELT(LR))	BKL	427
610	G(2*L+1)=-V(2*L)*(F1+F2*AK(L)*DELT(L))+V(2*L+1)*(1.-AK(LR)*DELT(LR))	BKL	428
	1))	BKL	429
620	G(M2)=-V(M2)*(1.-AK(MATM)*DELT(MATM))	BKL	430
	CALL SQUID	BKL	431
C	EVALUATE DEPOSITION BY FLUORESCENCE RADIATION	BKL	432

MSP=0	BKL 433
TAU= .0	BKL 434
J=1	BKL 435
ISPEC=0	BKL 436
DO 660 M=1,MATM	BKL 437
STOT=STTL(M)	BKL 438
AKK=AK(M)	BKL 439
STR=STRD(M)	BKL 440
AR=SABS(M)/RHOD(M)	BKL 441
RRZ=V(2*M-1)	BKL 442
CCZ=V(2*M)	BKL 443
EXX=EXK(M)	BKL 444
IF (J.EQ.MAT(M)) GO TO 630	BKL 445
MSP=MSP+1	BKL 446
DDP=CCZ*EXX+RRZ+DP1(MSP+1)	BKL 447
DDP1=(CCZ*EXX-RRZ+DP1(MSP+1))*AKK	BKL 448
SF=SURL(TAU)*SURR(TAUS-TAU)	BKL 449
DP(MSP)=DP(MSP)+0.25*SF*(DDP-DELT(M)*DDP1)	BKL 450
DP3(MSP)=DP3(MSP)+0.25*SF*(DDP+DELT(M)*DDP1)	BKL 451
ISPEC=ISPEC+1	BKL 452
SPEC(I,ISPEC)=SPEC(I,ISPEC)+SF*DDP	BKL 453
J=J+1	BKL 454
630 KK=LS(J)	BKL 455
ZZL=XP(MSP+1)	BKL 456
XTK=XT(J)	BKL 457
DO 650 K=1,KK	BKL 458
MTOT=MSP+K	BKL 459
ZZ=XP(MTOT)-ZZL	BKL 460
TAUT=TAU+ZZ*STR	BKL 461
EXKZ=EXP(-AKK*ZZ)	BKL 462
EXKR=EXP(AKK*(ZZ-XTK))	BKL 463
DDP=AB*(BBZ*EXKZ+CCZ*EXKR+DP1(MTOT))*SURL(TAUT)*SURR(TAUS-TAUT)	BKL 464
DP(MTOT)=DP(MTOT)+DDP	BKL 465
IF (NF.EQ.NZFL) GO TO 650	BKL 466
DO 640 N=NF1,NZFL	BKL 467
DPF=DDP*FRF(M,N)	BKL 468
FLSOUR(MTOT,N)=FLSOUR(MTOT,N)+DPF	BKL 469
640 DP(MTOT)=DP(MTOT)-DPF	BKL 470
650 CONTINUE	BKL 471
TAU=TAU+XT(J)*STR	BKL 472
MSP=MSP+LS(J)	BKL 473
J=J+1	BKL 474
IF (LOZ(J).GT.0) GO TO 660	BKL 475
MSP=MSP+1	BKL 476
DDP=CCZ+BBZ*EXX+DP1(MSP-1)	BKL 477
DDP1=(CCZ-BBZ*EXX-DP1(MSP-1))*AKK	BKL 478
SF=SURL(TAU)*SURR(TAUS-TAU)	BKL 479
DP(MSP)=DP(MSP)+0.25*SF*(DDP-DELT(M)*DDP1)	BKL 480
DP3(MSP)=DP3(MSP)+0.25*SF*(DDP+DELT(M)*DDP1)	BKL 481
ISPEC=ISPEC+1	BKL 482
SPEC(I,ISPEC)=SPEC(I,ISPEC)+SF*DDP	BKL 483
660 IF (LOZ(J).EQ.0) J=J+1	BKL 484
670 CONTINUE	BKL 485
680 DO 690 J=1,NSP	BKL 486

DPA(J)=DPA(J)*DF	BKL 487
DPT(J)=DPT(J)*DE	BKL 488
IF (DP3(J).LE.1. IF-6*DP(J)) DP3(J)=0.0	BKL 489
DP3(J)=DP3(J)*DF	BKL 490
600 DP(J)=DP(J)*DF	BKL 491
STFL=DP(NSP)	BKL 492
IF (PRNT.NE.0.) GO TO 740	BKL 493
PRINT 950, (VIC(I),I=1,10),CVR	BKL 494
MSP=1	BKL 495
DO 730 J=1,KL	BKL 496
NI=LS(J)	BKL 497
MSQ=MSP+NI-1	BKL 498
IF (LOZ(J).LE.0) GO TO 710	BKL 499
DO 700 I=MSP,MSQ	BKL 500
RAT=DP(I)/DPT(I)	BKL 501
DP2=0.418*DP(I)	BKL 502
700 PRINT 960, XP(I),DPA(I),DPT(I),DP3(I),RAT,DP(I),DP2	BKL 503
IF (LOZ(J+1).GT.0) PRINT 940, IV(4),ISTAR	BKL 504
GO TO 730	BKL 505
710 DO 720 I=MSP,MSQ	BKL 506
PRINT 970, XP(I),DP(I),DP3(I)	BKL 507
DP(I)=0.0	BKL 508
720 DP3(I)=0.0	BKL 509
730 MSP=MSP+NI	BKL 510
740 IF (PUNCH.EQ.0) GO TO 770	BKL 511
PUNCH 940, (VIC(LL),LL=1,10)	BKL 512
PUNCH 980, STFL	BKL 513
SUM=0.0	BKL 514
DO 750 I=1,NF	BKL 515
750 SUM=SUM+SPEC(I,ISPEC)	BKL 516
SUM=1.0/(DE*(SUM-.5*(SPEC(1,ISPEC)+SPEC(NF,ISPEC))))	BKL 517
DO 760 I=1,NF	BKL 518
760 DP1(I)=SUM*SPEC(I,ISPEC)	BKL 519
PUNCH 980, (E(I),DP1(I),I=1,NF)	BKL 520
770 IF (PLOTT.NE.0) GO TO 780	BKL 521
C PLOT DEPOSITION	BKL 522
CALL PLOUT (XP,DPA,NSP,7,1,2)	BKL 523
CALL PLOUT (XP,DPT,NSP,7,1,3)	BKL 524
CALL PLOUT (XP,DP3,NSP,7,1,7)	BKL 525
CALL PLOUT (XP,DP,NSP,7,1,4)	BKL 526
C PLOT SPECTRAL SENSITIVITIES AND SPECTRAL ESTIMATES	BKL 527
CALL PLOUT (E,SPSS,NF,7,MATM,5)	BKL 528
CALL PLOUT (F,SPSR,NF,7,MATM,6)	BKL 529
CALL PLOUT (E,SPEC,NF,6,ISPEC,8)	BKL 530
780 IRAD=1H1	BKL 531
N=3	BKL 532
IF (IERR.NE.0) GO TO 810	BKL 533
N=5	BKL 534
790 READ 940, NEXTJOB	BKL 535
IF (IABS(NEXTJOB).EQ.IABS(NJ(1))) GO TO 820	BKL 536
DO 800 I=2,N	BKL 537
IF (IABS(NEXTJOB).EQ.IABS(NJ(1))) GO TO 830	BKL 538
800 CONTINUE	BKL 539
PRINT 1020, IRAD,NEXTJOB	BKL 540

	IRAD=1H	BKL	541
810	IF (FATAL.FQ...) GO TO 790	BKL	542
C	DUMP BUFFER, CONSTRUCT END FRAME, AND ENDFILE PLOT TAPE	BKL	543
820	CALL DUMPER (ND1,ND2)	BKL	544
	CALL EXIT	BKL	545
830	ISLIP=(4-I)*(I-2)	BKL	546
	IF (I.LE.3) GO TO 10	BKL	547
	PRINT 840	BKL	548
	GO TO 30	BKL	549
C		BKL	550
840	FORMAT (1H1,30X,17HBUCKL CALCULATION)	BKL	551
850	FORMAT (3F8.0,8X,F8.0,8X,4F8.0)	BKL	552
860	FORMAT (25HODIMENSIONS EXCEEDED****,10A8/(1H ,A4,1H=,14))	BKL	553
870	FORMAT (14,5F10.4)	BKL	554
880	FORMAT (10HOCURRENT =,F12.5,9H CAL/SQCM//)	BKL	555
890	FORMAT (38H LAYER THICKNESS DIAM(CM) DENSITY ,8(10HZ WT.FR.)	BKL	556
	1)	BKL	557
900	FORMAT (2F8.0,2I5)	BKL	558
910	FORMAT (8(I2,F8.0))	BKL	559
920	FORMAT (14,F13.6,F10.3,F9.3,8(I3,F7.4)/36X,8(I3,F7.4))	BKL	560
930	FORMAT (14,F13.6,F10.3,3X,2A8)	BKL	561
940	FORMAT (1,A8)	BKL	562
950	FORMAT (1H1,10A8/16H0 INCIDENT FLUX =,E12.2//9X,5HX(CM),6X,5HAB,AB,BKL	BKL	563
	18X,6HAB,TOT,7X,8HNO FLUOR,3X,7HDEP/A,T,2X,11HDEP(CAL/GM),4X,7HDEP(BKL	BKL	564
	2MR),5X,8H+CURRENT,5X,8H-CURRENT)	BKL	565
960	FORMAT (F15.5,3E13.3,F9.3,2E13.3)	BKL	566
970	FORMAT (F15.5,74X,2E13.3)	BKL	567
980	FORMAT (2E15.7)	BKL	568
990	FORMAT (36H0THESE ELEMENTS ALLOWED TO FLUORESC/44H 2 FL-ENERGYBKL	BKL	569
	1 YIELD K-JUMP L-JUMP)	BKL	570
1000	FORMAT (1H0,10A8)	BKL	571
1010	FORMAT (F10.0)	BKL	572
1020	FORMAT (A1,10HNEXT JOB (,A8,34H) NOT RECOGNIZED OR NOT EXECUTABLE)	BKL	573
	END	BKL	574

SUBROUTINE COFF	CFF	1
COMMON/EVALU/F(2),B(20),C(20),D(20),H(20),V(20),G(20),M2	CFF	2
COMMON/COEFF/AK(10),DELTA(10),STTL(10),A(10),EXK(10),EXS(10),MATM,	CFF	3
1 XSKIP(1),YYZ	CFF	4
DO 1 II=1,M2	CFF	5
F(II)=0.	CFF	6
10 H(II)=0.	CFF	7
C(1)=-1.-AK(1)*DELTA(1)	CFF	8
D(1)=(-2.-C(1))*EXK(1)	CFF	9
G(1)=(1.+STTL(1)*DELTA(1))*A(1)	CFF	10
IF (MATM.EQ.1) GO TO 3,	CFF	11
MM1=MATM-1	CFF	12
DO 20 IL=1,MM1	CFF	13
IS=2*IL	CFF	14
IP=IL+1	CFF	15
X=XSKIP(IL)*2./YYZ	CFF	16
F1=(1.+0.2271*X)/(1.+1.0672*X*(1.+0.7621*X*(1.+0.2792*X)))	CFF	17
F2=(1.+0.13182*X)/(1.+0.0930*X*(1.+0.9530*X*(1.+0.15051*X)))	CFF	18
9(IS)=(1.-AK(IL)*DELTA(IL))*EXK(IL)	CFF	19
C(IS)=1.+AK(IL)*DELTA(IL)	CFF	20
D(IS)=-F1+F2*AK(IR)*DELTA(IR)	CFF	21
H(IS)=(-2*F1-D(IS))*EXK(IR)	CFF	22
G(IS)=-((1.-STTL(IL)*DELTA(IL))*EXS(IL)*A(IL)+(F1-F2*STTL(IR)*DELTA(IR)*A(IR))*A(IR)	CFF	23
IS=IS+1	CFF	24
F(IS)=(F1+F2*AK(IL)*DELTA(IL))*EXK(IL)	CFF	25
B(IS)=F1-F2*AK(IL)*DELTA(IL)	CFF	26
C(IS)=-1.-AK(IR)*DELTA(IR)	CFF	27
D(IS)=(-2.-C(IS))*EXK(IR)	CFF	28
20 G(IS)=-((F1+F2*STTL(IL)*DELTA(IL))*EXS(IL)*A(IL)+(1.+STTL(IR)*DELTA(IR)*A(IR))*A(IR)	CFF	29
IS=IS+1	CFF	30
30 B(M2)=(1.-AK(MATM)*DELTA(MATM))*EXK(MATM)	CFF	31
C(M2)=1.+AK(MATM)*DELTA(MATM)	CFF	32
G(M2)=-((1.-STTL(MATM)*DELTA(MATM))*EXS(MATM)*A(MATM)+A(MATM))	CFF	33
RETURN	CFF	34
END	CFF	35
	CFF	36

C	SUBROUTINE BIGGS	BIG	1
	READS CROSS-SECTION TAPE AND EVALUATES CROSS-SECTIONS	BIG	2
	DIMENSION A(331),EDGF(830),R(6),IEDGF(100),ZOA(100)	BIG	3
	COMMON/BICC/IZ,FARG,PF,AB,TOT	BIG	4
	COMMON/FLUOR/NZFL,IZFL(10),EKE(10),ELE(10)	BIG	5
	DATA(C1=1.14821),(C2=.061409),(C3=3.17146),(C4=.932779),	BIG	6
	1 (C5=.25720),(X0=511.006),(FL=.4406)	BIG	7
	E=FARG	BIG	8
	IF (E.LT.0.1) E=0.1	BIG	9
	KEY=)	BIG	10
10	NX=IEDGF(IZ)	BIG	11
	DO 20 M=1,2	BIG	12
	IF (E.LE.EDGE(NX)) GO TO 30	BIG	13
20	NX=NX+1	BIG	14
	PRINT 90, IZ,F	BIG	15
	RETURN	BIG	16
30	IF (KEY.NE.) GO TO 50	BIG	17
	NX=4*NX-4	BIG	18
	EO=1./F	BIG	19
	PE=0.0	BIG	20
	DO 40 M=1,4	BIG	21
	PE=PE+A(M+NX)*EO	BIG	22
40	EO=EO/E	BIG	23
	X=F/X0	BIG	24
	S=ZOA(IZ)*FL	BIG	25
	S=S/(((B(2)*X)+B(1))*X+1.)*X	BIG	26
	S=S/(((B(6)*X)+B(5))*X+B(4))*X+P(3))*X+1.0)	BIG	27
	AR=S+PF	BIG	28
	CT=ZOA(IZ)*FL	BIG	29
	CT=CT*(1.+X*(C1+X*C2))	BIG	30
	CT=CT/(1.+X*(C3+X*(C4+X*C5)))	BIG	31
	TOT=CT+PE	BIG	32
	RETURN	BIG	33
	ENTRY BIGGSF	BIG	34
	DO 80 I=1,NZFL	BIG	35
	KEY=1	BIG	36
	IZ=IABS(IZFL(I))	BIG	37
	IF (IZFL(I).GT.0) GO TO 70	BIG	38
	E=(FLOAT(IZ)/33.)*2.7	BIG	39
	ASSIGN 60 TO IGO	BIG	40
	GO TO 10	BIG	41
50	IF (ABS(EDGE(NX)-E).GT.ABS(E-EDGE(NX-1))) NX=NX-1	BIG	42
	GO TO IGO, (60,8)	BIG	43
60	ELE(I)=EDGE(NX)	BIG	44
70	E=(FLOAT(IZ)/11.)*2.2	BIG	45
	ASSIGN 80 TO IGO	BIG	46
	GO TO 10	BIG	47
80	EKE(I)=EDGF(NX)	BIG	48
	RETURN	BIG	49
	ENTRY BIGGSR	BIG	50
	READ (15) (A(I),I=1,3304)	BIG	51
	READ (15) (IEDGF(I),I=1,100)	BIG	52
	READ (15) (EDGF(I),I=1,826)	BIG	53
	READ (15) (ZOA(I),I=1,100)	BIG	54
	READ (15) (B(I),I=1,6)	BIG	55
	RETURN	BIG	56
C	90 FORMAT (25H CROSS-SECTION TROUBLE,Z=,13,3H E=,F8.4)	BIG	57
	END	BIG	58
		BIG	59

	SUBROUTINE INTENS (IERR)	INT	1
C	CALCULATES A COMPOSITE BLACK BODY SPECTRUM, READS A SPECTRUM FROM	INT	2
C	TAPE, READS SPECTRAL POINTS AT ENERGIES CALC IN MAIN PROGRAM,	INT	3
C	OR READS ENERGY AND SPECTRAL POINTS AND LINEAR INTERPOLATES	INT	4
	COMMON/SPECT/EMIN,DE,EMAX,NE,FLEVEL(400),L(400)	INT	5
	DIMENSION T(50),W(50),UU(200),VV(200)	INT	6
	DATA (MTAPF=15),(I1=1HB),(I2=3HS/F),(I3=1HS)	INT	7
	IERR=0	INT	8
	READ 18, IAM,FMT,NSEG	INT	9
	IF (ISIGN(IAM,I1).EQ.I1) GO TO 60	INT	10
	IF (ISIGN(IAM,I2).EQ.I2) GO TO 10	INT	11
	IF (ISIGN(IAM,I3).NE.I3) GO TO 110	INT	12
C	READ SPECTRUM FROM CARDS	INT	13
	READ FMT, (FLEVEL(I),I=1,NE)	INT	14
	IAM=8H MOTLEY	INT	15
	GO TO 150	INT	16
10	READ FMT, (UU(I),I=1,NSEG)	INT	17
	READ FMT, (VV(I),I=1,NSEG)	INT	18
	IAM=8H S/F	INT	19
	DO 50 J=1,NF	INT	20
	DO 40 I=2,NSEG	INT	21
	IF (UU(I)-E(J)) 40,20,30	INT	22
20	FLEVEL(J)=VV(I)	INT	23
	GO TO 50	INT	24
30	FLEVEL(J)=VV(I-1)+(E(J)-UU(I-1))*(VV(I)-VV(I-1))/(UU(I)-UU(I-1))	INT	25
	GO TO 50	INT	26
40	CONTINUE	INT	27
50	CONTINUE	INT	28
	GO TO 150	INT	29
C	READ BLACK BODIES	INT	30
60	READ 19, NBB,(W(I),T(I),I=1,NBB)	INT	31
	IF (EMIN.GT.0.) GO TO 90	INT	32
	TMAX=0.	INT	33
	TMIN=100.	INT	34
	DO 70 I=1,NBB	INT	35
	IF (T(I).GT.TMAX) TMAX=T(I)	INT	36
70	IF (T(I).LT.TMIN) TMIN=T(I)	INT	37
	EMIN=TMIN/12.	INT	38
	IF (EMIN.LT.0.1) EMIN=0.1	INT	39
	EMAX=TMAX*15.	INT	40
	DE=EMIN	INT	41
	IF ((EMAX-EMIN).GT.398.*DE) DE=(EMAX-EMIN)/398.	INT	42
	NE=(EMAX-EMIN)/DE+1.0	INT	43
	DO 80 I=1,NE	INT	44
80	E(I)=EMIN+DE*FLOAT(I-1)	INT	45
90	IAM=8H B.BODY	INT	46
	DO 100 I=1,NE	INT	47
	FLEVEL(I)=0.	INT	48
	DO 100 J=1,NBB	INT	49
100	FLEVEL(I)=FLEVEL(I)+W(J)*L(I)**3/((EXP(E(I)/T(J))-1.)*T(J)**4)	INT	50
	GO TO 150	INT	51
C	READ SPECTRUM FROM TAPE	INT	52
110	READ (MTAPF) NNM,NF	INT	53
	IF (EOF,MTAPE) 120,130	INT	54

120 PRINT 200, IAM	INT	55
RFWIND MTAPE	INT	56
IFRR=1	INT	57
RETURN	INT	58
130 IF (ISIGN(IAM,NNM).NE.NNM) GO TO 110	INT	59
READ (MTAPE) (FLEVEL(I),I=1,NE),EMIN,DE	INT	60
RFWIND MTAPE	INT	61
F(1)=EMIN	INT	62
DO 140 I=2,NE	INT	63
140 E(I)=FMIN+(I-1)*DF	INT	64
EMAX=E(NF)	INT	65
150 EE=0.	INT	66
DO 160 I=1,NF	INT	67
CIC=1.0	INT	68
IF (I.EQ.1.OR.I.EQ.NE) CIC=.5	INT	69
160 EE=EE+FLEVEL(I)*CIC	INT	70
EE=EE*DE	INT	71
DO 170 I=1,NE	INT	72
170 FLEVEL(I)=FLEVEL(I)/EL	INT	73
PRINT 210, IAM,EMIN,DE,EMAX	INT	74
RETURN	INT	75
C	INT	76
180 FORMAT (2A8,I8)	INT	77
190 FORMAT (11,7F10.5/(8F10.5))	INT	78
200 FORMAT (1H A8,19H NOT ON SPECT. TAPE)	INT	79
210 FORMAT (1X,A8,8HSPECTRUM,2X,5HEMIN=,F8.4,4H DE=,F8.4,6H EMAX=,F8.4	INT	80
1/)	INT	81
END	INT	82

	SUBROUTINE SQUID	SQD	1
C	SUBROUTINE TO SOLVE A QUIDIAGONAL SYSTEM OF EQUATIONS	SQD	2
	COMMON/EVALU/A(20),B(20),C(20),D(20),E(20),X(20),Y(20),N	SQD	3
	DIMENSION OM(20),RET(20),GAM(20),DEL(20)	SQD	4
10	OM(1)=C(1)	SQD	5
	RET(1)=D(1)/OM(1)	SQD	6
	DEL(2)=B(2)	SQD	7
	OM(2)=C(2)-DEL(2)*RET(1)	SQD	8
	IF (N.EQ.2) GO TO 30	SQD	9
	DO 20 I=3,N	SQD	10
	GAM(I-2)=F(I-2)/OM(I-2)	SQD	11
	RET(I-1)=(D(I-1)-DEL(I-1)*GAM(I-2))/OM(I-1)	SQD	12
	DEL(I)=B(I)-A(I)*RET(I-2)	SQD	13
20	OM(I)=C(I)-A(I)*GAM(I-2)-DEL(I)*RET(I-1)	SQD	14
30	X(1)=Y(1)/OM(1)	SQD	15
	X(2)=(Y(2)-DEL(2)*X(1))/OM(2)	SQD	16
	IF (N.EQ.2) GO TO 50	SQD	17
	DO 40 I=3,N	SQD	18
40	X(I)=(Y(I)-DEL(I)*X(I-1)-A(I)*X(I-2))/OM(I)	SQD	19
50	X(N-1)=X(N-1)-X(N)*RET(N-1)	SQD	20
	IF (N.EQ.2) RETURN	SQD	21
	DO 60 I=3,N	SQD	22
	K=N-I+1	SQD	23
60	X(K)=X(K)-RET(K)*X(K+1)-GAM(K)*X(K+2)	SQD	24
	RETURN	SQD	25
	END	SQD	26

C	SUBROUTINE PLOUT (X,Y,N,LY,IMULT,NDUM)	PLO	1
	CONSTRUCTS ALL PLOTS	PLO	2
	COMMON/PLTDAT/XMIN,XMAX,YMIN,YMAX	PLO	3
	DIMENSION X(400),Y(400,10),LAB(10)	PLO	4
	DATA (LAB=1H1,1H2,1H3,1H4,1H5,1H6,1H7,1H8,1H9,1H0)	PLO	5
	NTITLE=NDUM	PLO	6
	YMAX=0.	PLO	7
	XMIN=0.0	PLO	8
	XMAX=X(N)	PLO	9
	DO 10 J=1,N	PLO	10
	DO 10 I=1,IMULT	PLO	11
10	IF (Y(J,I).GT.YMAX) YMAX=Y(J,I)	PLO	12
	AL=ALOG10(YMAX)	PLO	13
	IF (AL.GT.0.) AL=AL+1.	PLO	14
	YMAX=10.0**INT(AL)	PLO	15
	YMIN=YMAX*10.**(-LY)	PLO	16
	IF (NTITLE.EQ.8) NTITLE=1	PLO	17
	CALL GRD (NTITLE,LY)	PLO	18
	DO 20 I=1,IMULT	PLO	19
20	CALL PLT (X,Y(1,I),N,LAB(I),IMULT)	PLO	20
	RETURN	PLO	21
	END	PLO	22

C	SUBROUTINE GRD (NTITLE,LY)	G66	1
	PLOTS GRID AND LABELS *****CDC 6600 VERSION*****	G66	2
	DIMENSION IR(10),T(28)	G66	3
	COMMON/PLTDAT/XYIN,XMAX,YMIN,YMAX	G66	4
	COMMON/TITLE/VIC(10)	G66	5
	DATA (T=8HSPECTRA ,8HCAL/SQ C,8HM/KEV VS,8H KEV ,8HAB-DEP, ,	G66	6
	1 8HAB-ATT ,8H CAL/GM ,8H ,8HAB-DEP, ,8HTOT-ATT ,	G66	7
	2 8H CAL/GM ,8H ,8HDEPOSITI,8HON DIR+S,8HCAT+FLUC,	G66	8
	3 8HR CAL/GM,8HDEP/DE ,8HLAYER FR,8HONT ,8H ,	G66	9
	4 8HDEP/DE ,8HLAYER BA,8HCK ,8H ,8HDEPOSITI,	G66	10
	5 8HON DIR+S,8HCAT CAL/,8HGM)	G66	11
	DATA (IX=0)	G66	12
	IF (IX.EQ.0) CALL ENTFLM (40)	G66	13
	IX=1	G66	14
	CALL SMXYV (0,1)	G66	15
	CALL DXDYV (1,XMIN,XMAX,DX,N,I,NX,10.,IERR)	G66	16
	IF (IERR.EQ.1) STOP 1	G66	17
	DY=1.	G66	18
	CALL GRIDIV (3,XMIN,XMAX,YMIN,YMAX,DX,DY,N,LY,-1,-LY,NX,LY)	G66	19
	DO 10 I=1,4	G66	20
10	CALL APRNTV (8,0,8,T(4*NTITLE-4+I),700+(I-1)*64,1010)	G66	21
	DO 20 I=1,10	G66	22
20	CALL APRNTV (0,-8,8,VIC(I),10,950-(I-1)*64)	G66	23
	RETURN	G66	24
	ENTRY DUMPER	G66	25
	IF (IX.NE.0) CALL EXTFLM (0)	G66	26
	RETURN	G66	27
	END	G66	28

C	SUBROUTINE PLT (X,YY,N,LAB,IMULT)	P66	1
	PLOTS AND IDENTIFIES A CURVE *****CDC 6600 VERSION*****	P66	2
	COMMON/PLTDAT/XL,XU,YL,YU	P66	3
	DIMENSION LG(2),IX(2),IY(2),X(1),YY(1)	P66	4
	YM=0.1*YL	P66	5
	DO 10 I=1,N	P66	6
10	IF (YY(I).LT.YM) YY(I)=YM	P66	7
	IYL=IYV(YL)	P66	8
	LG(1)=J	P66	9
	IX(1)=IXV(X(1))	P66	10
	IY(1)=IYV(YY(1))	P66	11
	IF (YY(1).GE.YL) GO TO 20	P66	12
	IY(1)=IYL	P66	13
	LG(1)=1	P66	14
20	DO 50 I=1,N	P66	15
	IX(2)=IXV(X(I))	P66	16
	IY(2)=IYV(YY(I))	P66	17
	LG(2)=0	P66	18
	IF (YY(I).GE.YL) GO TO 30	P66	19
	IY(2)=IYL	P66	20
	LG(2)=1	P66	21
30	IF (LG(1)*LG(2).NE.0) GO TO 40	P66	22
	CALL LINEV (IX(1),IY(1),IX(2),IY(2))	P66	23
40	IX(1)=IX(2)	P66	24
	IY(1)=IY(2)	P66	25
50	LG(1)=LG(2)	P66	26
	IF (IMULT.EQ.1) RETURN	P66	27
	NMIN=N/9	P66	28
	IF (NMIN.EQ.0) NMIN=N-1	P66	29
	IF (NMIN.EQ.0) NMIN=1	P66	30
	DO 70 J=1,N,NMIN	P66	31
	K=J	P66	32
60	IF (YY(K).GE.YL) GO TO 70	P66	33
	K=K+1	P66	34
	IF (K.GT.N) RETURN	P66	35
	GO TO 60	P66	36
70	CALL APLTV (1,X(K),YY(K),1,1,1,LAB,IERR)	P66	37
	RETURN	P66	38
	END	P66	39

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