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SPATIAL ASPECTS OF LOW- AND MEDIUM-ENERGY ELECTRON DEGRADATION IN N_2

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Abstract. Spatial (radial and longitudinal) yield spectra for electron energy degradation in molecular nitrogen gas for 25-eV to 10-keV incident electrons have been generated by using a Monte Carlo technique. These spatial yield spectra associated with the electron degradation process can be employed to calculate a 'yield' for any inelastic state at any position in the medium. These have been analytically represented in terms of a model containing three simple 'microplumes.' Five-dimensional yield spectra which contain the information about the polar angle of the electron have also been analytically represented within the framework of the microplume model. Aeronomical and radiological applications of our model are discussed.

Introduction

By generalizing the concept of yield spectra (YS) introduced by Green et al. [1977a, b] (to be referred to as GJG and GGJ, respectively), Jackman and Green [1979] have recently obtained numerical spatial (longitudinal (z) and radial (r)) yield spectra for electrons of initial energy ($0.1 \leq E_o \leq 5$ keV) incident along positive z axis in N_2 gas using a Monte Carlo technique. These four-dimensional yield spectra contain information regarding the yield of any excited state at any position in the medium. Recently, Green and Singhal [1979] have found a simple analytical representation of these four-dimensional YS in terms of a model using 'microplumes.' In the present work we (1) extend the Monte Carlo calculations to cover a broader range of incident electron energies (25 eV $\leq E_o \leq$ 10 keV); (2) represent the four-dimensional YS analytically for the entire energy range; (3) obtain an analytical representation of five-dimensional yield spectra which also includes the information about the polar angle (θ) of the electron at any position in the medium; and (4) include 'source' contributions to the yield spectra which are significant below a few hundred electron volts.

The model of four-dimensional YS is essentially the same as the one developed by Green and Singhal [1979] except that now a few of the microplume shape parameters have explicit energy dependence. The four-dimensional YS microplume model has been further generalized to incorporate the fifth degree of freedom, i.e., the polar angle of the electron at any position. With each four-dimensional microplume are associated a normalized angular distribution function, which is expressed as a combination of Henyey-Greenstein function and a second Legendre polynomial [Riewe and Green, 1978], and two parameters which depend on incident energy and position. In the present work we have slightly modified the multiple elastic scattering distribution (MESD) obtained by Kutcher and Green [1976] (to be referred to as KG) and used by Jackman and Green [1979] when the electron's energy falls below 30 eV during its degradation. Finally, the analytical yield spectra are compared with the Monte Carlo data at several values of E_o, r, and z.

Basic Definitions

The four- and five-dimensional YS which result after the incident electron of energy E_o and all its secondaries, tertiaries, etc. have been completely degraded in energy are represented by

$$U(E,r,z,E_o) = \frac{N(E,r,z)}{\Delta E \Delta z \Delta s} \ \mathrm{eV}^{-1}\ (\mathrm{gm/cm}^2)^{-3} \quad (1)$$

$$U(\theta,E,r,z,E_o) = \frac{N(E,r,z,\theta)}{\Delta\theta \Delta E \Delta z \Delta s}\ \mathrm{rad}^{-1}\ \mathrm{eV}^{-1}\ (\mathrm{gm/cm}^2)^{-3} \quad (2)$$

$$\Delta s = \pi\{(r + \frac{\Delta r}{2})^2 - (r - \frac{\Delta r}{2})^2\}$$

In (2), N(E, r, z, θ) is the total number of inelastic collisions that exist in the spatial interval $\Delta z \Delta s$ around (r, z), in the energy interval ΔE centered at E and polar angle interval $\Delta\theta$ centered at θ. Here, z is the longitudinal distance along the z axis, and $r = (x^2 + y^2)^{1/2}$ is the radial distance, both scaled by an 'effective range' $R(E_o)$. It is useful to represent the yield spectra by

$$U(E,r,z,E_o) = U_a(E,r,z,E_o)H(E_o-E-E_m) + \delta(E_o-E)D(r,z,E_o) \quad (3)$$

(following the notation of GJG and GGJ), where H is the Heaviside function with E_m the minimum threshold of the states considered, and $\delta(E_o - E)$ is the Dirac delta function which allows for the contribution of the source itself. A similar representation holds for the five-dimensional YS.

Monte Carlo Calculations

Numerical spatial yield spectra have been calculated for incident electron energy between 25 eV and 10 keV by using the Monte Carlo technique of Jackman and Green [1979]. However, in the present calculations the multiple elastic scattering distribution used below 30 eV has been slightly modified. Kutcher and Green [1976] have obtained distribution functions for the electrons arriving at a certain position (r, z) after a given number of elastic collisions, the electrons

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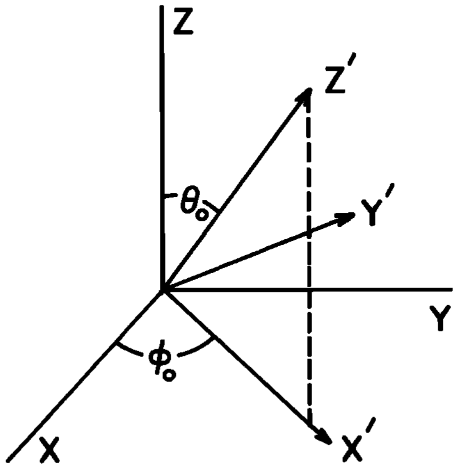

Fig. 1. Schematic of coordinate transformation.

entering initially along the positive z axis. In the Monte Carlo calculations the electron may be moving in the direction specified by (θ_o, ϕ_o) when its energy has fallen below 30 eV. Kutcher and Green [1975] results may therefore be applied only after making the coordinate transformation given by (see Fig. 1)

$$
\begin{aligned}
x &= x'\cos\theta_o \cos\phi_o - y'\sin\phi_o + z'\sin\theta_o \cos\phi_o \\
y &= x'\cos\theta_o \sin\phi_o + y'\cos\phi_o + z'\sin\theta_o \sin\phi_o \qquad (4) \\
z &= -x'\sin\theta_o + z'\cos\theta_o
\end{aligned}
$$

A Reparameterized Two-Dimensional Yield Spectrum

Green and Singhal [1979] have reparameterized the two-dimensional yield spectrum studied by GJG and GGJ in the form

$$U(E,E_k) = C_o + C_1\,\chi + C_2\,\chi^2 \qquad (5)$$

where C_0, C_1, and C_2 are external parameters and

$$\chi = \frac{E_k^{\Omega}}{E+L} \qquad (6)$$

where Ω and L are intrinsic parameters. E_k is incident electron energy in keV, and E is the spectral variable (in electron volts). In tests with (5) and (6) we have found it sufficient to let L = 1 eV and Ω = 0.585 for all gases. Table 1 gives the three remaining parameters, C_o, C_1, and C_2, for various gases. The similarity of the parameters from species to species confirms the near invariance of yield spectra. By using universal intrinsic parameters the problem of dealing with mixtures of gases becomes simply a matter of weighting the coefficients C_o, C_1, C_2, a somewhat simpler procedure than that used by Peterson et al. [1978].

In this work we will use (5) as an integral constraint upon the analytic microplume model for the four- and five-dimensional yield spectra generated by the Monte Carlo method.

The Plume Model of Four-Dimensional YS and Constraints

Following Green and Singhal [1979] we have represented the four-dimensional YS in the form

$$U_a(E,E_k,r,z) = \sum_{i=0}^{2} \frac{A_i}{R^3}\,\chi^i\,G_i(r,z) \qquad (7)$$

where each G_i is a microplume of the form

$$G_i(r,z) = \exp\left[-\left(\frac{\alpha_i r}{1+\delta_i z} + \beta_i^2 z^2 - \gamma_i z\right)\right] \qquad (8)$$

where r and z are the radial and longitudinal distances expressed in fractions of a scale factor or 'range' R given by (in grams per square centimeter)

$$R = R_o\,E_k^q + \tau \qquad (9)$$

The shape parameters α_2, β_2, and γ_2 for the forward microplume ($z \geq 0$) are somewhat dependent upon E_k in a fashion which may be represented by

$$\alpha_2 = \frac{(E_k/E_1)^{P_1}}{1 + (E_k/E_2)^{2P_1}} \qquad (10)$$

TABLE 1. Amplitude Parameters for the Two-Dimensional YS (Equation (5)), for Nine Atmospheric Gases

Gas	100 C_o	C_1	C_2
Ar	1.77	5.59	162.0
H_2	3.17	4.58	118.5
H_2O	1.97	6.03	117.4
O_2	1.08	6.15	177.0
N_2	1.66	5.04	169.0
O	1.40	5.02	246.9
CO	2.04	5.29	176.9
CO_2	1.49	6.28	199.4
He	1.34	4.17	125.0

TABLE 2. Shape and Amplitude Parameters for Four-Dimensional YS (Equations (8)-(14) and Equations (15)-(18)

	Forward	Backward
Shape parameter		
α_o	5.56	2.77
β_o	2.16	0.4
γ_o	6.41	d_{1b} = 2.31, E_6 = 21.7
δ_o	0.0	0.0
α_1	3.0	0.62
β_1	0.94	0.0
γ_1	1.16	E_7 = 0.32, p_2 = 1.71, E_8 = 0.022
δ_1	0.0	0.0
E_1 (α_{2f})	0.094	α_{2b} = 2.68
P_1 (α_{2f})	0.61	α_{2b} = 2.68
E_2 (α_{2f})	4.61	α_{2b} = 2.68
E_3 (β_{2f})	0.78	β_{2b} = 0.0
E_4 (β_{2f})	7.02	β_{2b} = 0.0
E_5 (γ_{2f})	0.65	γ_{2b} = 3.27
d_2 (γ_{2f})	0.11	γ_{2b} = 3.27
δ_2	0.0	-0.94
Amplitude Parameter		
k_o	0.058	
k_1	0.5	
R_e	3.55×10^{-8}	
t	0.56	
Scale factor		
q	1.766	
τ	2.0×10^{-7}	
R_o	3.4×10^{-6}	

$$\beta_2 = \frac{(E_k/E_3)^{P_1}}{1 + (E_k/E_4)^{2P_1}} \tag{11}$$

$$\gamma_2 = \frac{(E_k/E_5)}{1 + (E_k/E_4)^2} - d_2 \tag{12}$$

TABLE 3. Shape and Amplitude Parameters for the Four-Dimensional YS Source Microplume (Equations (21)-(23)

Parameter	Forward	Backward
E_9 (α_s)	0.097	2.9
P_3 (α_s)	0.71	2.9
E_{10} (α_s)	0.52	2.9
γ_s	3.53	-0.55
δ_s	0.42	0.1

The shape parameters γ_{ob} and γ_{1b} for the backward microplume ($z < 0$) are similarly given by

$$\gamma_{ob} = \frac{d_{1b}}{1 + (E_k/E_6)} \tag{13}$$

$$\gamma_{1b} = \frac{1 + (E_k/E_7)^{2P_2}}{(E_k/E_8)^{P_2}} \tag{14}$$

where E_1, E_2, ... , E_8 energy parameters are in keV and all other parameters are dimensionless. Their magnitudes are listed in Table 2.

To insure that our four-dimensional yield spectra go over to the two-dimensional yield spectra, we have imposed the following constraints:

$$A_{if} = \frac{C_i(1-k_i)}{I_{if}} \qquad i = 0,1 \tag{15}$$

TABLE 4. Parameters of Angular Distribution Functions Used in Five-Dimensional YS

Parameter	Value
E_{11}	0.0615
P_4	1.22
E_{12}	1.16
ℓ_2	5.20
ℓ_3	0.22
ℓ_4	3.00
ℓ_5	13.2
ℓ_6	2.19
E_{13}	1.28
E_{14}	0.0932
P_5	0.74
m_1	6.69
f_o	- 0.026
g_o	- 0.3

$$A_{ib} = \frac{C_i k_i}{I_{ib}} \tag{16}$$

so that

$$A_{if}\, I_{if} + A_{ib}\, I_{ib} = C_i \qquad i = 0,1 \tag{17}$$

where I_{if} and I_{ib} are the volume integrals

$$I_i = 2\pi \int_o^{\Lambda} \int_o^{\infty} G_i(r,z)rdrdz \tag{18}$$

Here, we identify the forward integral I_{if} when $\Lambda \to \infty$ and the backward integral I_{ib} when $\Lambda \to -\infty$.

We have only two parameters, k_o and k_i, at our disposal when adjusting the model for the 'primary' microplume amplitudes.

For the secondary microplume amplitudes we have found it necessary to introduce an energy dependence of the form

$$A_{2f} = \frac{C_2}{I_{2f}} \left[1 - \left(\frac{R_e}{R}\right)^t\right] \qquad A_{2b} = \frac{C_2}{I_{2b}} \left(\frac{R_e}{R}\right)^t \tag{19}$$

which gives us two adjustable parameters, R_e and t. Table 2 gives the microplume shape and amplitude parameters for the four-dimensional YS.

The Source Microplume

The source term $D(r, z, E_o)$ in (13) is expressed in the form

$$D(r,z,E_o) = \frac{A_s}{R^3} G_s \tag{20}$$

where

$$G_s = \exp\left[-\left(\frac{\alpha_s r}{1 + \delta_s z} + \gamma_s z\right)\right] \tag{21}$$

The shape parameter α_s for the forward source microplume has the explicit energy dependence of the form

$$\alpha_s = \frac{1 + (E_k/E_9)^{2P_3}}{(E_k/E_{10})^{P_3}} \tag{22}$$

The amplitude A_s is constrained by

$$A_{sf} = \frac{(1-k_s)}{I_{sf}} \tag{23a}$$

and

$$A_{sb} = \frac{k_s}{I_{sb}} \tag{23b}$$

where

$$I_s = 2\pi \int_o^{\Lambda} \int_o^{\infty} G_s(r,z)rdrdz \tag{24}$$

and $k_s = k_o$. Table 3 gives the parameters for the source microplume.

Five-Dimensional Yield Spectra

In some aeronomical problems the polar angle distribution associated with the electron spectrum also plays an important physical role. We have incorporated this additional degree of freedom by generalizing (7) of four-dimensional YS in the form

$$U(\theta,E,r,z,E_o) = \sum_{i=0}^{2} \frac{A_i}{R^3} G_i(r,z)\, Q_i \tag{25}$$

where Q_i's are the normalized angular distribution functions

$$\int_o^{\pi} Q_i d\theta = 1 \qquad i = 0,\ 1,\ 2 \tag{26}$$

Q's have been represented with the aid of a combination of a Henyey-Greenstein function [Riewe and Green, 1978] and a second Legendre polynomial ($\mu = \cos\theta$)

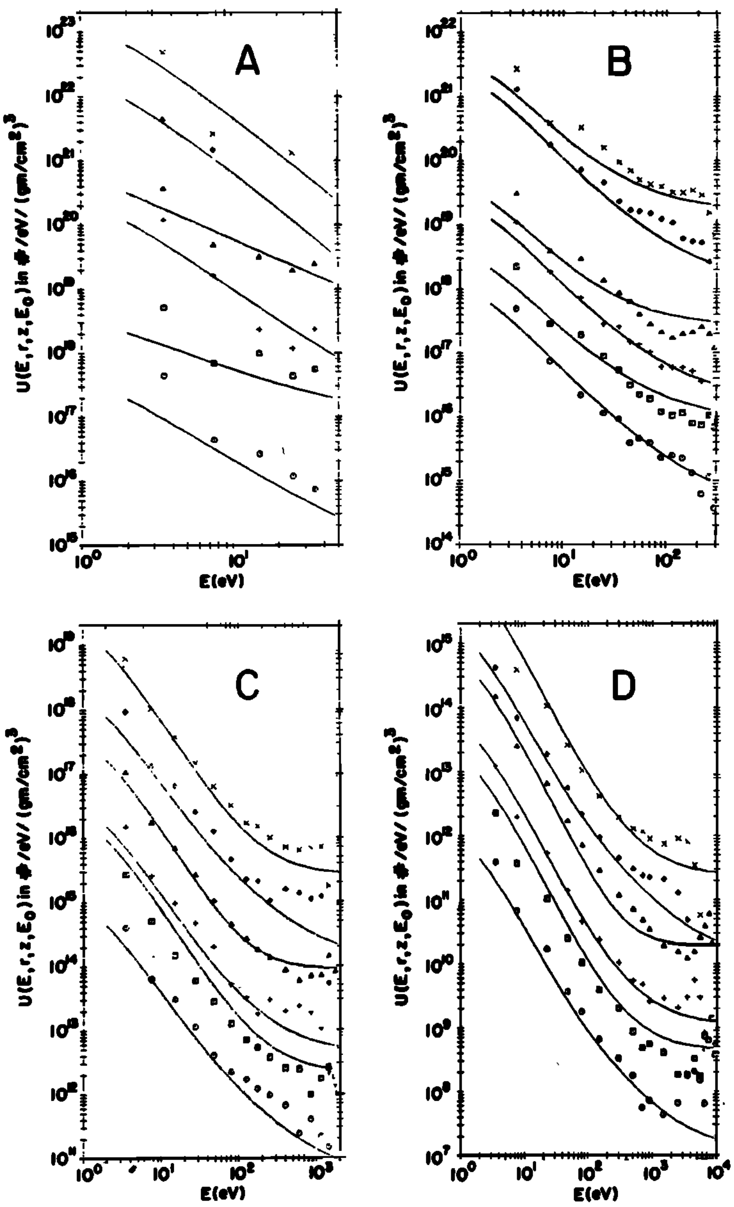

Fig. 2. The four-variable spatial yield spectrum U (E, r, z, E_o) is plotted as a function of E at four incident energies E_k (in keV): (a) 0.05, (b) 0.3, (c) 2, and (d) 10. The Monte Carlo calculations are represented by symbols (see Table 5), and the analytic fit using equation (7) is represented by the solid line.

$$Q_1 = Q_0 = \frac{(1-g^2)}{2}\left[\frac{1}{(1+g^2-2g\mu)^{3/2}} + \frac{f}{2}(3\mu^2-1)\right]\sin\theta \tag{27a}$$

and

$$Q_2 = (1 - w'(E,E_o)\tfrac{1}{2}(3\mu^2-1))/(\pi - \tfrac{\pi}{4}\, w'(E,E_o)) \tag{27b}$$

The forward microplumes f and g are functions of the electron's energy and position as given below:

$$g = w(E,E_o)\ \exp\left[\frac{-\ell_1 r^2}{(1+\ell_2 z^2)}\right] - \ell_3\ \exp\left[-\ell_4 z^2(1+r^2)\right] \tag{28}$$

$$f = -\frac{1}{(1+g^2+2|g|)^{3/2}}\, w(E,E_o)\ \{1-\exp(-\ell_5 r^2)\} \tag{29}$$

$$w(E,E_o) = \frac{\exp\{m_1(\frac{E}{E_o} - m_2)\}}{1 + \exp\{m_1(\frac{E}{E_o} - m_2)\}} \tag{30}$$

and w' is obtained by multiplying E/E_o in the expression for $w(E,E_o)$ by $E_k^{\ell_6}$.

We thus have eight adjustable parameters, two of which are explicit functions of primary energy E_k:

TABLE 5. Monte Carlo Calculations (Figure 2)

Symbol	Fig. 2a E_k=0.05 keV	Fig. 2b E_k=0.3 keV	Fig. 2c E_k=2 keV	Fig. 2d E_k=10 keV
Square				
r	0.63	0.45	0.33	0.3
z	0.21(1)	0.15(1)	0.11(1)	0.1(1)
Circle				
r	1.93	1.08	0.99	0.9
z	0.21(1)	0.15(1)	0.11(1)	0.1(1)
Triangle				
r	0.63	0.45	0.33	0.3
z	1.93(400)	0.45(10)	0.55(10)	0.4(10)
Plus				
r	1.93	1.08	0.99	0.9
z	1.93(800)	0.45(20)	0.55(20)	0.5(20)
Cross				
r	0.63	0.45	0.33	0.3
z	3.85(3x10^5)	1.08(10^3)	1.22(10^3)	1.3(10^3)
Diamond				
r	1.93	1.08	0.99	0.9
z	3.85(10^5)	1.08(2x10^3)	1.22(2x10^3)	1.3(2x10^3)

The numbers in parentheses show the values by which the yield spectrum has been multiplied.

$$\ell_1 = \frac{(E_k/E_{11})^{p_4}}{1 + (E_k/E_{12})^{2p_4}} \qquad m_2 = \frac{1 + (E_k/E_{13})^{2p_5}}{(E_k/E_{14})^{p_5}} \tag{31}$$

For the backward microplumes f and g are found to be independent of position and energy of the electron. Thus

$$Q_{0b} = \frac{(1-g_o^2)}{2}\left[\frac{1}{(1+g_o^2-2g_o\,\mu)^{3/2}} + \frac{f_o}{2}(3\mu^2-1)\right]\sin\theta \tag{32}$$

and

$$Q_{1b} = \frac{f_o}{2}(3\mu^2-1)\sin\theta + \tfrac{1}{2}\sin\theta \qquad Q_{2b} = \frac{1}{\pi} \tag{33}$$

We thus have only two adjustable parameters, g_o and f_o.

The five-dimensional YS for the source term (20) is written in the form (see (23))

$$D(\theta,r,z,E_o) = \frac{A_s}{R^3} G_s Q_s \tag{34}$$

where Q_s is the normalized source angular distribution function which for forward microplume is given by

$$Q_s = \{2\pi P_{EX}\exp(-\ell_5 r^2) + (1-\exp(-\ell_5 r^2))\,(\tfrac{1}{2}-\tfrac{1}{4}(3\mu^2-1))\}\sin\theta \tag{35}$$

Here P_{EX} is the phase function for elastic scattering given by (4) of Jackman and Green [1979].

For backward source microplume we use the angular distribution function given by Q_{0b} (equation (32)).

Table 4 gives the microplume parameters for our best composite model to date for the five-dimensional YS including the source term. In Figures 2-3 we compare the present analytical representations of four- and five-dimensional YS based upon the microplume model with the Monte Carlo data.

Discussion and Conclusions

Since the concepts of two-dimensional YS (GJG and GGJ) and three- and four-dimensional YS (JG) and the treatment of the multiple elastic scattering problem (KG) are new and perhaps unfamiliar to the reader, we will attempt to clarify the purposes of our model. Essentially, the problem of characterizing the basic nature of the electron energy deposition process in a form which can be utilized to predict the spatial and energy dependence of all types of yields is an exceedingly difficult one. While there has been recognition that the ultimate explanation must be given in terms of detailed atomic (or molecular) cross sections (DACS), it is only recently that realistic attempts have been made (see JG and GJG for references) to use such a base. The reluctance to use a DACS base has in part been due to the intrinsic complexity of such inputs and in part upon the expectation that the results could be communicated only in the form of a large mass of computer output or graphs. Essentially, our microplume model suggests that the major features of most of the important results not only for N_2 but for all light gases can be explained in terms of three forward microplumes, three backward microplumes, and a source microplume, each of which can be characterized by a few intrinsic shape pa-

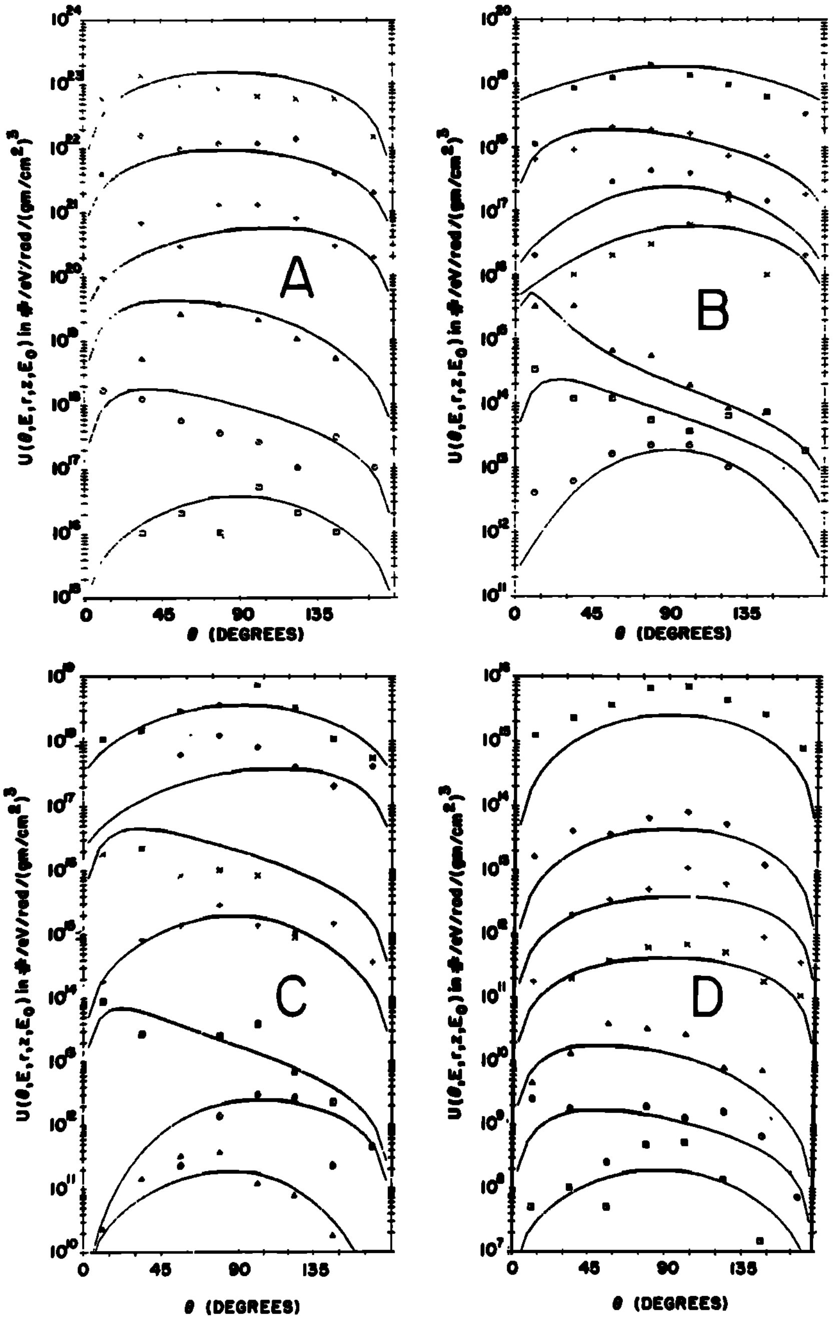

Fig. 3. The five-variable spatial yield spectrum $U(\theta, E, r, z, E_0)$ is plotted as a function of θ at four incident energies E_k (in keV): (a) 0.1, (b) 1, (c) 2, and (d) 10. The Monte Carlo calculations are represented by symbols (see Table 6), and the analytic fit using equation (25) is represented by the solid line.

rameters. Using this model we not only substantially reduce the number of adjusted parameters needed to characterize spatial yield spectra but we boil down exceedingly complex quantities into simple components.

In the present work we have, with some sacrifice of simplicity, broadened the range of applicability of the microplume model of Green and Singhal [1979]. Previously, they were able to use fewer parameters for the incident energy range from 0.1 to 5 keV. To extend the range from 25 eV to 10 keV while retaining the basic model, we have made several of the microplume parameters energy dependent. In addition, the other new features of the present work, i.e., the characterization of the source contribution and the polar angle distribution have necessitated the enlargement of our parameter set. Thus the increase of parameters has been more than compensated for by the extra accuracy and information contained in the representation.

As to overall fits of our analytic expressions to the Monte Carlo results, it should be noted that the magnitudes of our four-variable yield spectra (see Figure 2) range over eight decades and the five-variable yield spectra (see Figure

TABLE 6. Monte Carlo Calculations (Figure 3)

Symbol	Fig. 3a E_k=0.1 keV	Fig. 3b E_k=1 keV	Fig. 3c E_k=2 keV	Fig. 3d E_k=10 keV
Square				
E	89.5	700	1400	7000
r	0.69	0.1	0.11	0.5
z	0.14	0.1	0.11(10)	0.1(2)
Circle				
E	89.5	700	1400	7000
r	0.14	0.9	0.55	0.1
z	0.69	0.5(2)	0.11(5)	0.1(2)
Triangle				
E	89.5	700	1400	7000
r	0.69	0.1	0.55	0.5
z	0.69(500)	0.9	0.55(0.1)	0.5(50)
Plus				
E	40	300	700	1400
r	0.69	0.1	0.55	0.5
z	0.14(10^4)	0.1(10^4)	0.55(10^3)	0.5(10^4)
Cross				
E	40	300	700	1400
r	0.14	0.9	0.11	0.5
z	0.69(10^5)	0.1(10^4)	0.55(2x10^3)	0.7(10^3)
Diamond				
E	40	300	150	150
r	0.69	0.9	0.9	0.9
z	1.25(2x10^5)	0.5(2x10^4)	0.1(10^6)	0.5(10^5)
Star				
E		67.5	150	150
r		0.5	0.5	0.5
z		0.5(10^5)	0.5(10^6)	0.5(10^6)

The numbers in parentheses show the values by which the yield spectrum has been multiplied.

3) range over nine decades. Thus 'accuracy of fit' must be viewed in a logarithmic rather than linear perspective. Within this context we might note that our fits are not of uniform quality over the entire range of incident (E_k) and spectral (E) energies. Thus the fits are poorer at low incident energies ($E_k \sim 0.05$) and at high incident energies for the large spectral energies than at most other E_k, E combinations. The error introduced by these departures, however, should tend to cancel, particularly when integrating over E to obtain populations, since our analytic expressions usually vary above and below the Monte Carlo 'data.' It is believed, however, that our representations should give sufficiently accurate results for purposes of applications to planetary atmospheres, astrophysical problems, radiological physics, etc., in which the experimental data are still not very precise. Furthermore, alternative theoretical descriptions are either not available or exceedingly cumbersome to apply.

Finally, we should note that our present microplume model of four-dimensional YS can already be used for the study of many basic biophysical mechanisms in radiological physics and many processes in upper atmospheric physics. It can be applied to the study of the low- and medium-energy electron initiated processes in gases, in weakly magnetic planets such as Mars and Venus, or in comets. The five-dimensional YS which also contain information about the polar angle of the electron at any position in the medium can be applied to the study of the problem of bremsstrahlung generation by auroral electrons and the problem of backscattering. To apply the present yield spectra for magnetic planets such as Jupiter and Earth, one must also consider the effect of magnetic field. This will form the subject matter of subsequent communication. We are also planning to test our model by generating Monte Carlo data for other gases.

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