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by

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A MONTE CARLO TRANSPORT ROUTINE FOR THE

"U. S. STANDARD ATMOSPHERE" (1962) TO AN ALTITUDE OF 90 KILOMETERS

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ABSTRACT

Following the 1962 U. S. Standard Atmosphere report (NASA, USAF, USWB), the earth's atmosphere to 90 km is subdivided into eight horizontal zones, in each of which the temperature is assumed a linear function of altitude. The barometric equation is integrated on this basis to obtain formulas for the numerical density function, which closely approximates the tabulation of the report cited. Further integration then yields Monte Carlo routines for the usual "distance to collision" decision. A flow diagram is included, with all required constants. The method, which is more realistic than an earlier one based on a single exponential density, may be used in conjunction with any neutron and/or photon code, but was intended primarily for the existing (MCP) photon code, which allows for pair production, coherent and incoherent scattering with appropriate form factors, and fluorescence subsequent to photo electric absorption. A series of such problems was run on the CDC-7600, with a monoenergetic photon point-source (.5, 1.5, 5.0 MeV) at 50 km altitude, directed vertically downward, using the U. S. Standard Atmosphere, and for comparison, an exponential atmosphere assumed in earlier studies. The direct transmission is tabulated, and some discussion of the results is included. In general, the U. S. Atmosphere allows less penetration with a factor of 1/2 or less not uncommon.

I. THE DENSITY FUNCTION

For a column of air above the earth's surface S (Fig. 1), of area A, and height $Z^* = 90$ km,

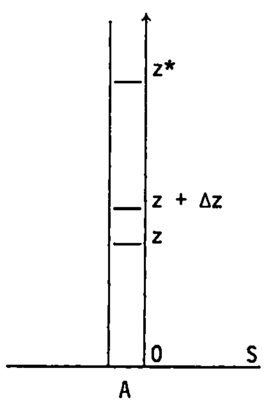


Fig. 1

we assume a force variation

$$F(z) = F(z + \Delta z) + \rho(A\Delta z)g$$

and hence a pressure gradient

$$dp/dz = -\rho(z)g(z) \qquad (1)$$

where $p = \bar{n}kT$, $\rho = (M/N_o)\bar{n}$, $g = g_o/[1+(z/R_E)]^2$, $\bar{n}$ being the molecular numerical density (see Table I for notation). The constant percentage composition (cf. [1]) for $z<z^*$ insures the constancy of the average molecular weight M, and of the ratio

$$C = n(z)/\bar{n}(z) \quad ; \quad z<z^*$$

of atomic to molecular density.

TABLE I

k = 1.380527×10^{-16} erg/°K, Boltzmann constant

M = 28.9644 gm, av. "molecular wt." of air, constant for $z < 90$ km

N_0 = 6.02257×10^{23}, Avogadro's number/mole

g_0 = 980.665 cm/sec^2, earth surface gravity (GM_E/R_E^2)

R_E = 6371 km, mean earth radius

R = $N_0 k$ = 8.31432×10^7 erg/°K mole, gas constant

K = R/Mg_0 = 2.92713×10^3 cm/°K

AIR COMPOSITION
($z < z^*$)

Molecular Component	% Numerical Composition
N_2	78.084
O_2	20.9476
Ar	.934
CO_2	.0314
Ne	.001818

Substitution in (1) yields the differential equation

$$d(\bar{n}T)/(\bar{n}T) = -\,Mg\,dz/RT$$

from which we obtain the basic density-temperature relation

$$\bar{n}(z) = \bar{n}_i (T_i/T(z)) \exp\left[-\int_{z_i}^{z} Mg(z)dz/RT(z)\right] \qquad (2)$$

where $z_i < z^*$ is an arbitrary altitude, and

$$\bar{n}_i = \bar{n}(z_i) \quad , \quad T_i = T(z_i) \quad .$$

Following [1], we suppose the function $T(z)$ defined by a broken line of 8 segments, as indicated in Fig. 2, and given explicitly in Table II. We have taken the exact vertices of [1; Table I 4e], but assumed the T-segments linear in altitude z, rather than in "geopotential altitude," to facilitate computation. However, we use in (2), for each of the 8 zones, the exact value of $\bar{n}_i = \bar{n}(z_i)$ tabulated in [1], and, to achieve "goodness of fit," take for $g(z)$ a constant value $\bar{g}_i$ (Table III) such that integration of (2) gives $\bar{n}(z_{i+1}) = \bar{n}_{i+1}$. This procedure results in a function $\bar{n}(z)$ closely approximating the tabulation in [1].

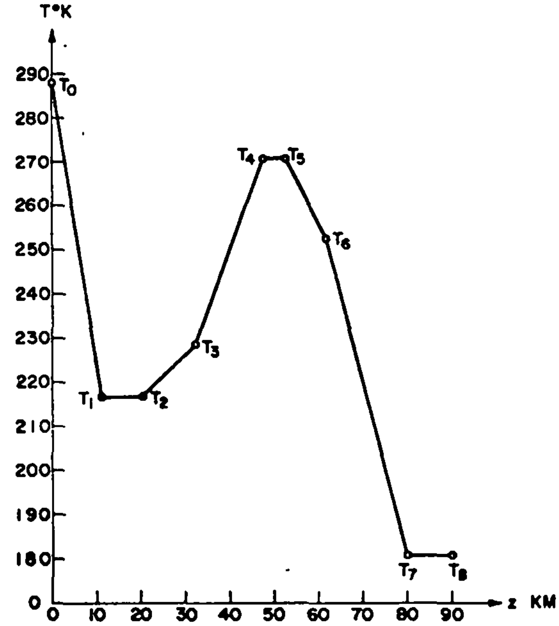


Fig. 2

The integral in (2) is easily evaluated for each of the two types of temperature function $T(z)$:

F. Flat case. $T(z) \equiv T_i$ on $z_i \leq z < z_{i+1}$. From (2), we find

$$\bar{n}(z)/\bar{n}_i = \exp[-(z-z_i)/H_i] \qquad (3)$$

$$H_i = K_i T_i (\text{cm}) \quad ; \quad K_i = R/M\bar{g}_i \quad (\text{cm}/°\text{K})$$

S. Slant case. $T(z) = T_i + \Gamma_i(z-z_i)$ on $z_i \leq z < z_{i+1}$. Integration in (2) yields

$$\bar{n}(z)/\bar{n}_i = \left[1+U_i(z-z_i)\right]^{-H_i-1} \qquad (4)$$

$$U_i = \Gamma_i/T_i(\text{cm}^{-1}),\ H_i = 1/K_i\Gamma_i,\ K_i = R/M\bar{g}_i(\text{cm}/°\text{K})$$

Here, the slope Γ_i is in °K/cm, and H_i is demensionless. These results are collected in Table II.

II. DISTANCE TO COLLISION

A beam of N "projectile" particles, of energy E, passing through a thickness dl of air of atomic density $n(z(\ell))$, and "macroscopic cross section" $\sigma = \sigma(E)$ (see below), suffers an attenuation

TABLE II

C_0	$0 = z_0 \leq z < z_1$ (cm)	$T = T_0 + \Gamma_0(z-z_0)$	$\bar{n} = \bar{n}_0[1 + U_0(z-z_0)]^{-H_0-1}$
C_1	$z_1 \leq z < z_2$	$T \equiv T_1$	$\bar{n} = \bar{n}_1 \exp[-(z-z_1)/H_1]$
C_2	$z_2 \leq z < z_3$	$T = T_2 + \Gamma_2(z-z_2)$	$\bar{n} = \bar{n}_2[1 + U_2(z-z_2)]^{-H_2-1}$
C_3	$z_3 \leq z < z_4$	$T = T_3 + \Gamma_3(z-z_3)$	$\bar{n} = \bar{n}_3[1 + U_3(z-z_3)]^{-H_3-1}$
C_4	$z_4 \leq z < z_5$	$T \equiv T_4$	$\bar{n} = \bar{n}_4 \exp[-(z-z_4)/H_4]$
C_5	$z_5 \leq z < z_6$	$T = T_5 + \Gamma_5(z-z_5)$	$\bar{n} = \bar{n}_5[1 + U_5(z-z_5)]^{-H_5-1}$
C_6	$z_6 \leq z < z_7$	$T = T_6 + \Gamma_6(z-z_6)$	$\bar{n} = \bar{n}_6[1 + U_6(z-z_6)]^{-H_6-1}$
C_7	$z_7 \leq z < z_8 = 9.10^6$	$T \equiv T_7$	$\bar{n} = \bar{n}_7 \exp[-(z-z_7)/H_7]$

	STORAGE						
i	z_i cm	$F_i = \bar{n}_0/\bar{n}_i$	H_i	U_i cm^{-1}	T_i °K	$\bar{n}_i$ cm^{-3}	Γ_i °K/cm
0	0	1	- 5.2558396	-.0225187992 - 05	288.15	2.5471 + 19	-6.488792 - 05
1	11.019 + 05	3.36611	6.3726298 + 05 cm	-	216.65	7.5669 + 18	0
2	20.063 + 05	13.9148	34.162943	.0045779714 - 05	216.65	1.8305 + 18	.9918175 - 05
3	32.162 + 05	92.6252	12.2011335	.0120942095 - 05	228.65	2.7499 + 17	2.765341 - 05
4	47.350 + 05	858.101	8.0474151 + 05 cm	-	270.65	2.9683 + 16	0
5	52.429 + 05	1613.01	-17.0817899	-.0072589562 - 05	270.65	1.5791 + 16	-1.9646365 - 05
6	61.591 + 05	4878.66	- 8.5407577	-.0154854764 - 05	252.65	5.2209 + 15	-3.9124056 - 05
7	79.994 + 05	61213.65	5.4302657 + 05 cm	-	180.65	4.1610 + 14	0
(8)	90.000 + 05	-	-	-	180.65	6.5910 + 13	-

Note: $x \pm y$ means $x \times 10^{\pm y}$

TABLE III

i	$\bar{g}_i/g_0$
0	.998269
1	.995134
2	.991810
3	.987621
4	.984449
5	.982329
6	.978096
7	.973775

$$dN/N = -\sigma n(z(\ell))d\ell$$

and hence satisfies the "decay" law

$$N(\ell) = N(0) \exp\left[-\int_0^\ell \sigma n(z(\ell))d\ell\right] \quad .$$

We therefore regard the exponential as the probability $Q(\ell)$ of transmission through distance ℓ, and $P(\ell) = 1-Q(\ell)$ as the distribution function for collision at distance $\leq \ell$. When $n(z(\ell))$ is well defined for all $\ell < \infty$, and $Q(\infty) = 0$, setting a random number

$$r = Q(\ell) = \exp\left[-\int_0^\ell \sigma n(z(\ell))d\ell\right] \qquad (5)$$

serves to determine the distance ℓ to collision in an infinite medium. This simple rule is subject to various qualifications in the present case, as indicated below.

In what follows, we suppose the earth to be flat ($z^* << R_E$), and the atmosphere above it divided into the 8 altitude zones of Table II. Thus a projectile, travelling a distance $\ell > 0$ in the direction

$\Omega = (u,v,w)$ from a point of departure $P = (X,Y,Z)$ in the i-th such zone, will then be at an altitude (Fig. 3)

$$z(\ell) = Z + w\ell$$

where the atomic density is

$$n(z(\ell)) = C\bar{n}(z(\ell)) = C\bar{n}_i \cdot \bar{n}(z(\ell))/\bar{n}_i = C\bar{n}_0(\bar{n}_i/\bar{n}_0)$$
$$\times \bar{n}(z(\ell))/\bar{n}_i = (n_0/F_i)\ \bar{n}(Z+w\ell)/\bar{n}_i\ ;\ F_i \equiv \bar{n}_0/\bar{n}_i \tag{6}$$

(see Table II).

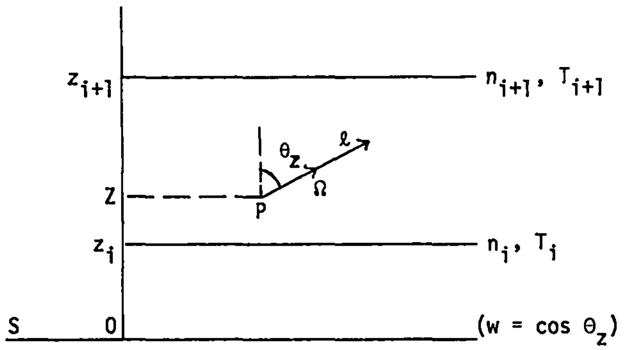


Fig. 3

Existing codes allow computation of the quantity

$$\lambda = 1/\sigma n_0 \tag{7}$$

where n_0 is the atomic density of air at sea level, and

$$\sigma = \sum f_j \sigma_j(E)$$

is its "macroscopic cross section," the f_j defining its fractional <u>atomic</u> composition. In evaluating (5), we will therefore use (6), (7) to express

$$\sigma n(z(\ell)) = (\sigma n_0/F_i)\ \bar{n}(z(\ell))/\bar{n}_i = (\lambda F_i)^{-1}$$
$$\times \bar{n}(Z+w\ell)/\bar{n}_i \tag{8}$$

in terms of λ, the stored F_i, and the density ratios of (3), (4).

It remains to show how a random number r is used to determine the distance ℓ to collision, in each of the cases F, S above.

<u>F. Flat case.</u> Substitution of (8), (3) in (5) gives

$$r = Q(\ell) = \exp\left[-(\lambda F_i E)^{-1} \int_0^\ell e^{-W\ell}\, d\ell\right] \tag{9}$$

$$E = \exp(Z - z_i)/H_i \quad , \quad W = w/H_i$$

We are faced with the following possibilities.

<u>F° (w = 0)</u> . From (9),

$$r = Q(\ell) = \exp\left[-(\lambda F_i E)^{-1}\ell\right]$$

and we simply set

$$\ell = L;\ L \equiv -\lambda F_i E\ \ell n\ r,\ 1 \geq r > 0,$$
$$0 \leq \ell < \infty \quad . \tag{10}$$

For $w \neq 0$, (9) becomes

$$r = Q(\ell) = \exp\left[-(\lambda F_i E W)^{-1}\ (1 - e^{-W\ell})\right] \tag{11}$$

or $\quad \ell = -W^{-1}\ \ell n(1 - WL) \qquad (12)$

<u>F^-(w < 0)</u> . In (11), $Q(\infty) = 0$, and (12) defines ℓ on $0 \leq \ell < \infty$ for $1 \geq r > 0$

<u>F^+(w > 0)</u> . For $W > 0$, (11) shows that there is a non-zero probability

$$Q(\infty) = \exp\left[-(\lambda F_i E W)^{-1}\right] > 0 \tag{13}$$

of transmission through an infinite medium with <u>no</u> collision, and therefore only random numbers $r > Q(\infty)$ determine collisions with $\ell < \infty$. In this case, we therefore have the alternatives

<u>$F^+\ell$ ($1 \geq r > Q(\infty)$)</u>, $0 \leq WL < 1$, $0 \leq \ell < \infty$ from (12),

<u>$F^+\infty$ ($Q(\infty) \geq r > 0$)</u>, $1 \leq WL$, $\ell = \infty$.

$\underline{S.\ \ \text{Slant case.}}$ Substitution of (8), (4) in (5) yields

$$r = Q(\ell) = \exp\left[-(\lambda F_i)^{-1} \int_0^{\ell} (V + U_i w\ell)^{-H_i - 1} d\ell\right] \quad (14)$$

$$V \equiv 1 + U_i(Z - z_i) > 0$$

Note here that $|H_i| > 1$, and V is the ratio T/T_i at the point of departure P. We again consider the possibilities.

$\underline{S°(w = 0).}$ From (14),

$$r = Q(\ell) = \exp\left[-\left(\lambda F_i V^{H_i+1}\right)^{-1} \ell\right]$$

and we therefore set

$$\ell = V^{H_i+1} L;\ L \equiv -\lambda F_i\ \ell n\ r \geq 0,\ 1 \geq r > 0, \qquad (15)$$
$$0 \leq \ell < \infty$$

For $w \neq 0$, we obtain from (14),

$$r = Q(\ell) = \exp\left\{-(\lambda F_i U_i w H_i)^{-1} \times \left[V^{-H_i} - (V + U_i w\ell)^{-H_i}\right]\right\} \qquad (16)$$

$$\text{or } \ell = \left[(V^{-H_i} - LU_i wH_i)^{-1/H_i} - V\right] \Big/ U_i w \qquad (17)$$

with L as in (15).

In considering the remaining cases, it is well to bear in mind that: n(z) is a positive decreasing function of z; U_i, H_i both have the sign of Γ_i; and $Q(\ell)$ is a decreasing function of ℓ for $w \geq 0$, with $Q(0) = 1$.

$\underline{S^{--}(w < 0,\ \Gamma_i < 0).}$ As in case F^-, we have $Q(\infty) = 0$, and (17) defines ℓ on $0 \leq \ell < \infty$ for $1 \geq r > 0$.

$\underline{S^{++}(w > 0,\ \Gamma_i > 0)}$. This is analogous to Case F^+, since

$$Q(\infty) = \exp\left[-(\lambda F_i U_i wH_i)^{-1}\ V^{-H_i}\right] > 0$$

and there are the alternatives

$\underline{S^{++}\ell(1 \geq r > Q(\infty))}$, $0 \leq LU_i wH_i < V^{-H_i}$, $0 \leq \ell < \infty$ from (17),

$\underline{S^{++}\infty(Q(\infty) \geq r > 0)}$, $V^{-H_i} \leq LU_i wH_i$, $\ell = \infty$.

In these cases, T is increasing with ℓ, on the line of flight. In the remaining cases, the opposite is true, and neither $n(\ell)$ nor $Q(\ell)$ is defined for $T/T_i = V + U_i w\ell < 0$. However, since T/T_i remains positive throughout zone i, we may proceed as follows:

$\underline{S^{-+}(w < 0,\ \Gamma_i > 0}$. $Q(\ell)$ is defined for $0 \leq \ell < \ell^*$, where $V + U_i w\ell^* = 0$ and $Q(\ell^*) = 0$. Hence (17) defines ℓ on $0 \leq \ell < \ell^*$ for $1 \geq r > 0$.

$\underline{S^{+-}(w > 0,\ \Gamma_i < 0)}$. $Q(\ell)$ is defined on $0 \leq \ell < \ell^*$ as before, but now

$$Q(\ell^*) = \exp\left[-(\lambda F_i U_i wH_i)^{-1}\ V^{-H_i}\right] > 0.$$

This leads to the alternatives

$\underline{S^{+-}\ell(1 \geq r > Q(\ell^*))}$, $0 \leq LU_i wH_i < V^{-H_i}$, $0 \leq \ell < \ell^*$ from (17)

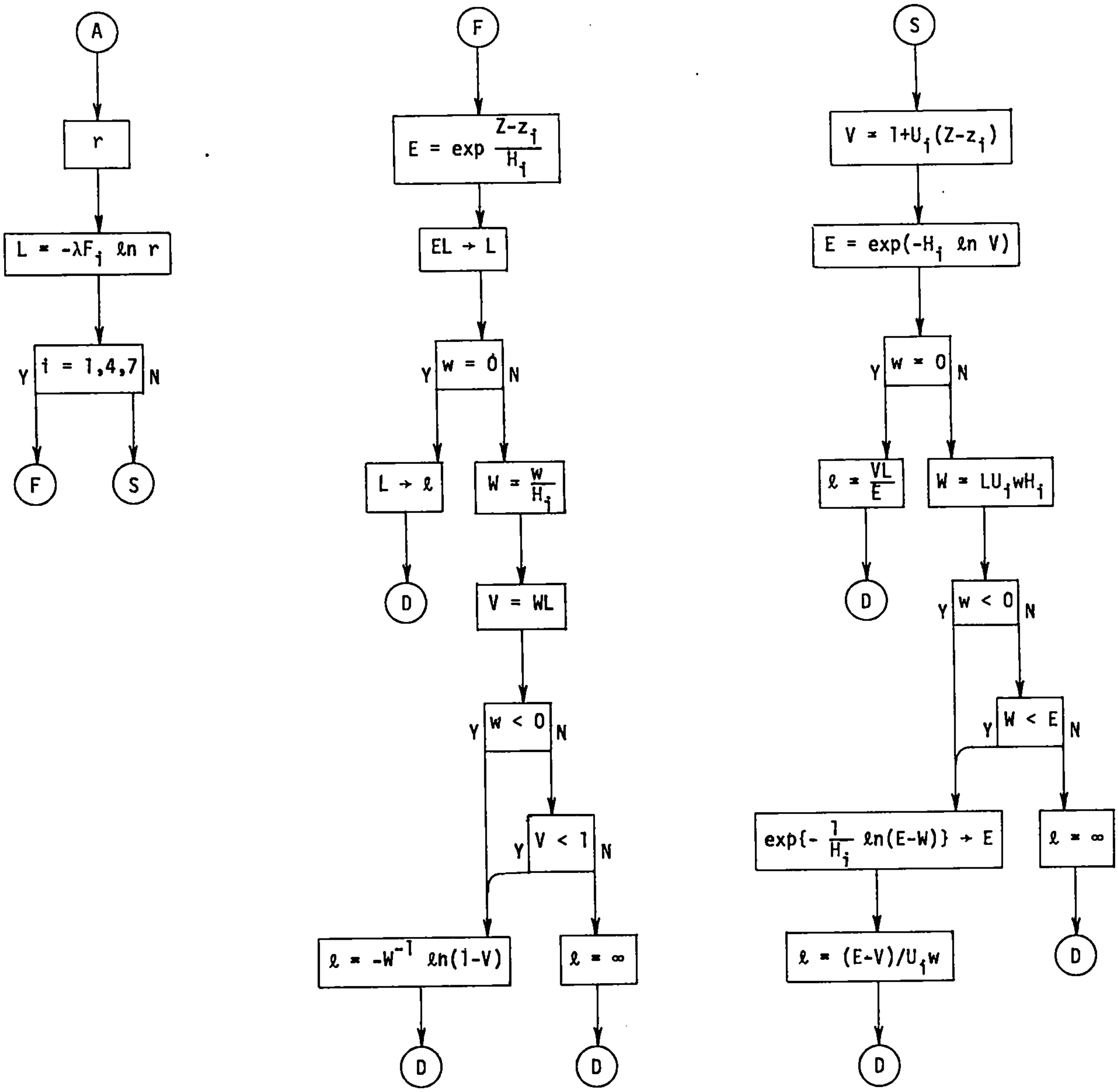
$\underline{S^{+-}\infty(Q(\ell^*) \geq r > 0)}$, $V^{-H_i} \leq LU_i wH_i$, $\ell = \infty$.

Note that the setting $\ell = \infty$ is only a Monte Carlo strategy which forces transport to the boundary.

III. ROUTINE FOR "DISTANCE ℓ TO COLLISION"

We enter from the free path routine of the regular code at the "λ-point," with $\lambda = \sigma n_0$ (cf. II), the point of departure parameters P = (X, Y, Z), Ω = (u,v,w), and the index i = 0,...,7 of the zone in which P lies. For storage, see Table II.

The exit (D) refers to the "collision or escape" routine of the regular code, which compares the distance ℓ with that to the boundary of the current cell, along the line of flight. In case of collision within the cell, the code resumes the free path at the "λ-point," from which (A) was entered. Escape connotes either escape from the system, or passage to an adjacent cell, and entry of the free path routine to obtain λ for the new cell. In the



present application, λ does not change from cell to cell, but only upon change of energy due to collision.

IV. COMPARISON OF U. S. WITH AN EXPONENTIAL ATMOSPHERE

Two series of 3 problems each were run on the CDC-7600, the first assuming the "U. S. Standard Atmosphere" treated above, the second a pure "exponential atmosphere", essentially that employed in [2].

Both series involved an infinite slab geometry, of height 90 km, with monoenergetic photon point-sources (.5, 1.5, 5.0 MeV) at altitude 50 km, directed vertically downward. A 3-component atmosphere of N_2, O_2, Ar was assumed, with molecular abundancies 78.111%, 20.955%, .934%, respectively. This corresponds to a ratio $n/\bar{n} = C = 2(.78111) + 2(.20955) + (.00934) = 1.99066$ and hence to a fractional atomic composition

$$f_N = .78478 \qquad f_O = .21053 \qquad f_A = .00469 \quad .$$

The source cross sections per atom, and the f-averaged macroscopic cross sections σ used, are shown in Table IV.

TABLE IV

E MeV	barns/atom σ_N	σ_0	σ_A	σ	Ser. I λ U.S. cm.	Ser. II λ Exp. cm.
.5	2.02465	2.31671	5.26680	2.10134	.0938559 + 05	.0776914 + 05
1.5	1.20219	1.37286	3.11429	1.24709	.1581466 + 05	.1309096 + 05
5.0	.63640	.73610	1.85800	.66311	.2974214 + 05	.2461974 + 05

The λ of Series I is given by $\lambda = 1/n_0\sigma$, where $n_0 = \bar{n}_0 C = 2.5471 \times 10^{19} \times 1.99066 = 5.0704 \times 10^{19}$ atoms/cm^3 is the sea level U. S. atomic density.

In Series II, a single exponential density

$$n(z) = n_0^* e^{-z/H};\ H = 6.7 \times 10^5 \text{cm},\ 0 \leqslant z < 9 \times 10^6 \text{cm}$$

was assumed. The λ of Series II in the table above is defined as $\lambda = 1/n_0^* \sigma$, with $n_0^* = 6.12535 \times 10^{19}$ atoms/cm^3 at sea level. This corresponds to an electron density of 10^{20} cm^{-3} at 10 km, as postulated in [2]. The above value of H is also that used in [2].

The direct transmissions, for a vertical path through the 8 zones, may be computed at once from the formulas (11), (16) for $Q(\ell)$, and are given for 5 MeV in Table V, for each of the lower 5 zones. Also included is the analogous transmission for the path from source altitude $z = 50 \times 10^5$ cm to the lower boundary z_4 of its zone. These numbers were realized with good precision in the Monte Carlo runs.

The analogous transmissions Q(E) for energies $E \neq 5$ MeV are easily obtained from the relation $Q(E) = Q^{\sigma(E)/\sigma(5)}$. The $\sigma(E)$ used in the problem are given in Table IV. The analogue of Table V for source E = 1.5, 0.5 MeV are given in Tables VI, VII.

TABLE V

SOURCE E = 5 MeV

	Q U.S. At.	Q Exp. At.		Q U.S. At.	Q Exp. At.
$50 \to z_4$	.9912	.9925	$50 \to z_4$	.9912	.9925
$z_5 \to z_4$	.98535	.9877	-	-	-
$z_4 \to z_3$	.8069	.8182	$50 \to z_3$	.7998	.8121
$z_3 \to z_2$	.2725	.3203	$50 \to z_2$	.2179	.2601
$z_2 \to z_1$	.008023	.0204	$50 \to z_1$	.00175	.00531
$z_1 \to z_0$	2.62 - 10	2.91 - 10	$50 \to z_0$	~ 0	~ 0

TABLE VI

SOURCE E = 1.5 MeV

	Q U.S.	Q Exp.		Q U.S.	Q Exp.
$50 \to z_4$	.9835	.9859	$50 \to z_4$	.9835	.9859
$z_5 \to z_4$	.9726	.9770	-	-	-
$z_4 \to z_3$	.6680	.6857	$50 \to z_3$	.6570	.6760
$z_3 \to z_2$	.08672	.1175	$50 \to z_2$	.05698	.07943
$z_2 \to z_1$	1.145 - 04	6.622 - 04	$50 \to z_1$	6.524 - 06	5.260 - 05
$z_1 \to z_0$	9.55 - 19	1.16 - 18	$50 \to z_0$	~ 0	~ 0

TABLE VII

SOURCE E = 0.5 MeV

	Q U.S.	Q Exp.		Q U.S.	Q Exp.
$50 \to z_4$	.9724	.9764	$50 \to z_4$	.9724	.9764
$z_5 \to z_4$	.9543	.9616	-	-	-
$z_4 \to z_3$	.5067	.5295	$50 \to z_3$	.4927	.5170
$z_3 \to z_2$	.016245	.02711	$50 \to z_2$	.008004	.01402
$z_2 \to z_1$	2.286 - 07	4.399 - 06	$50 \to z_1$	1.830 - 09	6.167 - 08
$z_1 \to z_0$	4.33 - 31	6.04 - 31	$50 \to z_0$	~ 0	~ 0

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