NUS CORPORATION

NUS – 722

MID–TERM REPORT FOR MODIFICATION OF CODES NUALGAM AND BREMRAD

For

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION
GODDARD SPACE FLIGHT CENTER
GREENBELT, MARYLAND

CONTRACT NAS5–11781

By

J. J. STEYN

&

R. HUANG

August 1970

NUS CORPORATION
4 Research Place
Rockville, Maryland 20850

08

NUS–722

MID–TERM REPORT FOR MODIFICATION OF CODES NUALGAM AND BREMRAD

For

Goddard Space Flight Center
Greenbelt, Maryland

NASA Contract Number: NAS5–11781

By

J. J. Steyn & R. Huang

August 1970

NUS CORPORATION
4 Research Place
Rockville, Maryland 20850

Approved: ______________________
E. A. Saltarelli
Vice President and Technical Director
Plant Engineering

TABLE OF CONTENTS

SUMMARY

This contract mid-term progress report discusses the development of modifying the existing gamma photon Monte Carlo radiation transport code NUALGAM and converting the existing analytic bremsstrahlung generation code BREMRAD. The NUALGAM modifications for the IBM/360 digital computer include transport phenomena such as buildup factors, albedos, fluorescent radiation emission and simulation of scintillation detector response. The BREMRAD conversion includes internal storage of frequently used coefficient data, logic modification and translation for operation on the IBM/360 digital computer.

LIST OF FIGURES

LIST OF TABLES

1. INTRODUCTION

This mid-term progress report, prepared for the National Aeronautics and Space Administration, Goddard Space Flight Center, by NUS CORPORATION, under contract NAS5-11781, discusses the progress of modifying the existing code NUALGAM [(1)] and converting the existing code, BREMRAD [(2)]. The NUALGAM computer code was developed by NUS for NASA/GSFC. The BREMRAD code was developed by H. H. Van Tuyl [(3)] for a UNIVAC computer and subsequently modified for specific NASA/GSFC requirements by NUS; it was also translated by NUS for operation on the GSFC IBM-7094 digital computer.

2. WORK PROGRESS

2.1 TASK I

The code BREMRAD work scopes under contract Task I, consisted of modification of existing code version logic, internal storage of frequently used data tabulations and a translation for operation on the IBM-360/91 digital computer. This task has been completed by NUS and reported to NASA/GSFC in Technical Report NUS-TM-NA-109, February, 1970 [(4)]. An operating code version and sample problem in accordance with the noted report has been delivered to GSFC.

2.2 TASK II

The code NUALGAM modifications under contract Task II, consist of deriving a code or group of codes for the NASA/GSFC IBM-360/91 digital computer to predict various gamma photon and fast neutron transport phenomena. The derivation uses code NUALGAM as the precursor. The transport phenomena to be predicted includes such as buildup factors, albedos, fluorescent radiation generation and spectral distribution of absorbed energy for scintillators. The work also includes a generalization of the geometry and composition of the transport medium as well as a statistical study and the utilization of magnetic tape storage of data and code versions. Contract Task II work scope is detailed as follows:

> Modify the IBM-360 Fortran IV Monte Carlo code NUALGAM to include the following:
>
> a. prediction of fluorescent radiation transport,
> b. generalization of the transport and source medium geometry,
> c. statistical evaluation of calculated predictions,
> d. generalization for multi-layer media transport,
> e. computation of number, energy, and exposure buildup factors,
> f. computation of number, energy, and exposure albedos,
> g. input of cross-section data and code versions from tape,
> h. generation of sodium-iodide (NaI (Tl)) scintillation crystal response function distributions as a function of energy and geometry within and outside the isotope general energy range,
> i. prediction of fast neutron transport,
> j. generation of organic scintillator fast neutron response function distributions:

A more detailed report on the work progress of each of the foregoing items is now presented:

Item A.

Work on the design of the logic for this item: fluorescent radiation transport, has been initiated.

Item B.

Work on the design of the logic for this item: generalization of transport and source geometry, has been initiated. Work on point isotropic, disc isotropic and parallel beam and uniform cylindrical source emission has been completed. These will be attached to code versions for optional implementation.

Item C.

Work on this item: code prediction statistics, has been initiated.

Item D.

Work on the design and logic of this item: multi-layer transport media, has been completed. The logic has been satisfactorily encoded into the codes under items (e), (f) and (h).

Item E.

Work on this item: gamma photon number, energy and exposure dose buildup factors has been initiated. A computer code NUGAM1 has been designed and encoded. This code, which is now undergoing debugging, will be similar in capability to NUGAM2, described below. It will be fully described in the final report to the present work.

An early version of NUGAM1 has been incorporated into code SØSC, developed by NUS for NASA/GSFC [5].

Item F.

Work on this item: gamma photon number, energy and dose albedos, has been initiated and is almost completed. The code NUGAM2 is now operational and being checked out. This code can determine photon albedos as a function of incident angle and energy, material atomic number and compositions, laminar disposition, material lateral dimension and thickness and incident radiation beam geometry, ie. parallel beam, point source, etc.

NUGAM2 is presently coded for cylindrical media of length L and radius R as shown in Figure 1. Axial incidence is obtained by highly collimating the incident parallel beam case. The code separately tallies single and double back scattering. Some preliminary examples of this codes usefulness are given below.

The number of gamma photons backscattered as a function of L and within a radius d located on the backscatter plane, were determined to ascertain the limitations of the albedo technique. Total number albedos for 1.25 and 0.662 MeV normal photon incidence are given in Figures 2 and 3 as a function of both d (open points) and L (solid points), in units of mean free path λ (E), with Z as a parameter. A saturation albedo for Z = 13 is reached a $d = d_{\infty} \sim 3 \lambda$ and 2.5λ, for E = 1.25 and 0.662 MeV, respectively; for Z = 82, $d_{\infty} < 0.25 \lambda$ at both energies. It was found that half of the backscattered photons emerged within a characteristic distance, $d = d_{1/2}$, typical values of which are given in Table I in units of λ (E). Analogous half and saturation thicknesses were observed to be approximately 85% of the $d_{1/2}$ and d_{∞} values. The total number albedos could be approximated as a function of either d or L, by the exponential relationship form reported by others.[6.7] The saturation total number, energy and exposure albedos were found to be in excellent agreement with the Monte Carlo and in good agreement with the experimental data of reference (8).

Figure 4 shows the code calculated total number albedo as a function of normally incident photon energy, with atomic number as the parameter. The references in this figure are from reference (8). Figure 5 gives examples of the total number albedo as a function of the angle of incidence θ_o (with respect to the scattering medium outward normal). For the sake of the expected value at $\theta_o = 90°$, the albedos in this figure are multiplied by $\cos\theta_o$.

Figure 6 shows the ratio of the single-scatter to total-scatter total number albedo as a function of energy. In this figure $\alpha_{N_{ss}}/\alpha_{N_T}$ is plotted as a function of E_o, with atomic number as a parameter. Typical single and double scatter to total number albedo ratios α_{ss} and α_{ds}, determined in this study are given in Table II. It can be seen that multiple (>2) scattering in lead accounts for only ~1% of the number albedo at E = .662 MeV. The Monte Carlo single scattering data were substantiated by a double numerical integration of the analytic differential transport equation, indicating that albedos for high Z media may be readily approximated by this method. The analytic transport equation used in this evaluation was defined, with reference to Figure 7, as

$$\alpha_{N_{ss}} = 2\pi r_e^2 N_e \int_0^L e^{-\mu_o z} \left\{ \int_{\theta=0}^{\theta_{max}} \sigma(\theta, E_o)\, e^{-\mu_s z/\cos\theta} \sin\theta \, d\theta \right\} dz,$$

where

r_e = classical electron radius,

= 2.8183×10^{-3} (cm),

N_e = number of electrons/cm^3,

$\sigma(\theta, E_o)$ = Klein-Nishina Function (cm^2/ster.-electron),

μ_O = total cross-section for E_O (cm^{-1}),

μ_S = total cross-section for E_S (cm^{-1}),

E_O = incident photon energy (MeV),

$$E_S = \frac{E_O}{1 + (E_O/0.511)(1-\cos\theta_S)} \;;\; \theta_S = \pi - \theta, \text{ (MeV)}.$$

Table III presents a comparison of analytic and NUGAM2 Monte Carlo single scatter albedos. The agreement can be seen to be excellent for low atomic number and as poor as 15% 'error' for high atomic number. The deviation expresses to a large extent, the statistical error in the Monte Carlo data. The analytic equation was encoded and solved using Simpson's Rule in code SSALB.

Code SSALB is considered as the basis of a very useful engineering code for radiation backscatter analysis. For example, Table III indicates $(\alpha_{N_{SS}})$anal. = 0.0656 for Z = 13 and E_O = 0.662. Table II gives R_{SS} = 0.24, thus using the analytic single scatter albedo the total albedo may be estimated as α_N = (0.0656/0.24) = 0.274, which is in very good agreement with 0.26 in Figure 3. This approach based on Monte Carlo data, offers an economical method in subsequent engineering analysis.

Item G.

Work on this item: input of data and codes from magnetic tape, though underway, will only be carried to completion as the contract items involved are completed.

Item H.

Work on this item: a sodium-iodide (NaI (Tℓ)) scintillation crystal photon response simulation code, has been partially completed. The NaI (Tℓ) code: NUGAM3, is now semi-operational. By this it is meant that at present it can generate response spectra for incident photon energies in the energy range up to ~1.5 MeV. The logic for the pair production phenomenon and for detector cladding is presently being developed.

A comparison of NUGAM3 results with those of reference (9) for a photon energy E = 0.662 MeV , a 3" x 3" NaI cylindrical crystal and two different source geometries was

	NUGAM3	REFERENCE (9)
Point Source at 10cm:	$P(E) = 0.568$	$= 0.562$
	$\epsilon(E) = 0.616$	$= 0.619$
Broad Parellel Beam	$P(E) = 0.587$	$= 0.578$
	$\epsilon(E) = 0.876$	$= 0.888$

where P(E) and $\epsilon(E)$ are photofraction and interaction officiency, respectively.

Item I.

Work on this item: Monte Carlo prediction of fast neutron transport in finite media, has been initiated and will proceed through the second half of the contract period.

Item J.

Work on this item: generation of organic scintillator response to fast neutrons, has been initiated and is proceeding. Work on this item is reliant on item I.

3. WORK PROGRAM FOR SECOND TERM

Throughout the second and remaining term of this contract, the work program already described will be carried to completion. The codes developed will be made operational on the NASA/GSFC 360/91 digital computer and then delivered to the Technical Officer along-with descriptive and user documentation, in accord with the contract requirements.

REFERENCES

1. STEYN, J. J. and STRAHL, J. T.,"NUALGAM - A Monte Carlo Code to Predict the Angular Energy Escape of Gamma Photons from Cylindrical Sources", NUS-536, NUS Corporation (1969).

2. STEYN, J. J., "Code BREMRAD for the IBM-7094 Computer," NUS-TM-NA-91, NUS Corporation (1968).

3. VAN TUYL, H. H., "BREMRAD - A Computer Code for External and Internal Bremsstrahlung Calculations," HW-83784, Hanford Laboratories (1964).

4. RUDY, G. C., "Code BREMRAD for the IBM-360 Computer", NUS-TM-NA-109, NUS Corporation (1970).

5. STEYN, J. J., and HUANG, R. "Final Report for Unmanned Spacecraft RTG Shield Optimization Study", NUS-679, NUS Corporation (1970).

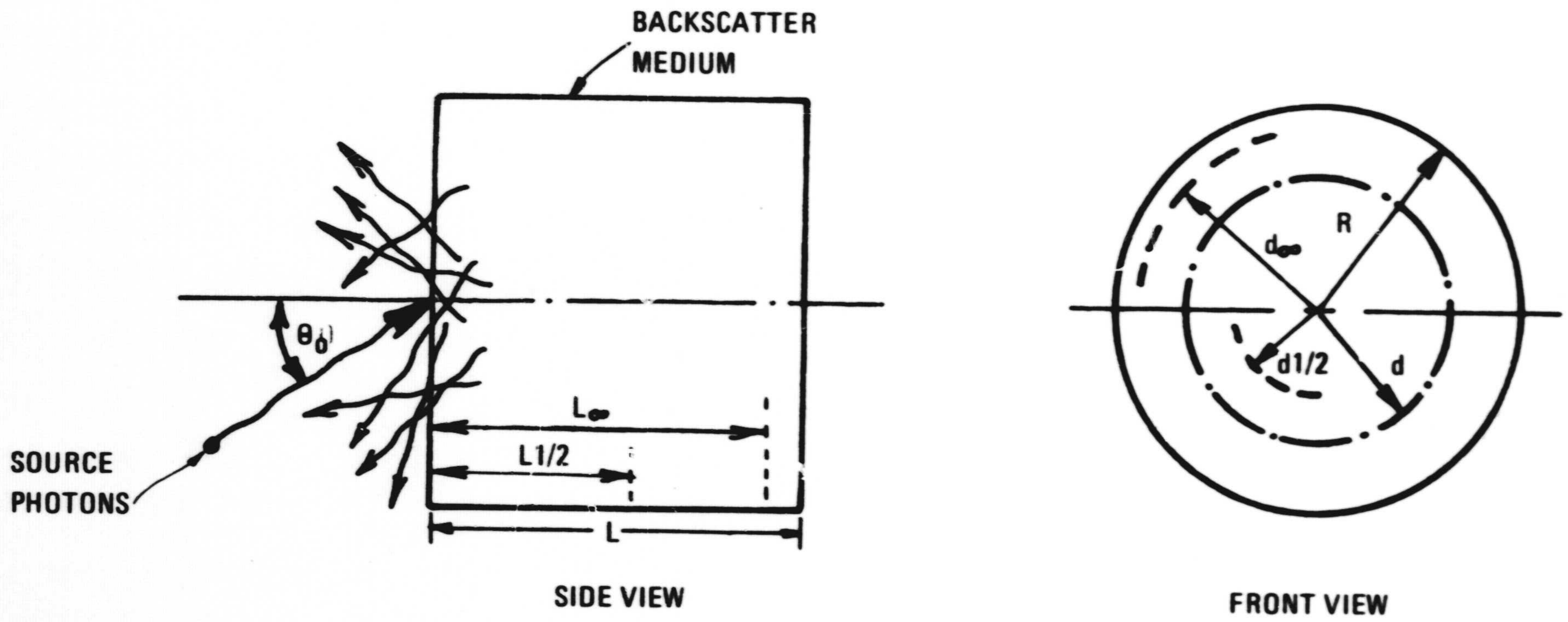
6. HYODO, R., "Backscattering of Gamma Rays", Nuclear Sci. and Eng., 12, 178 (1962).

7. BULATOV, B.P. and GARUSOV, E.A., "Co^{60} and Au^{198} Gamma Ray Albedos of Various Materials", J. Nucl. Energy, Part A: Reactor Science, 11, 159 (1960).

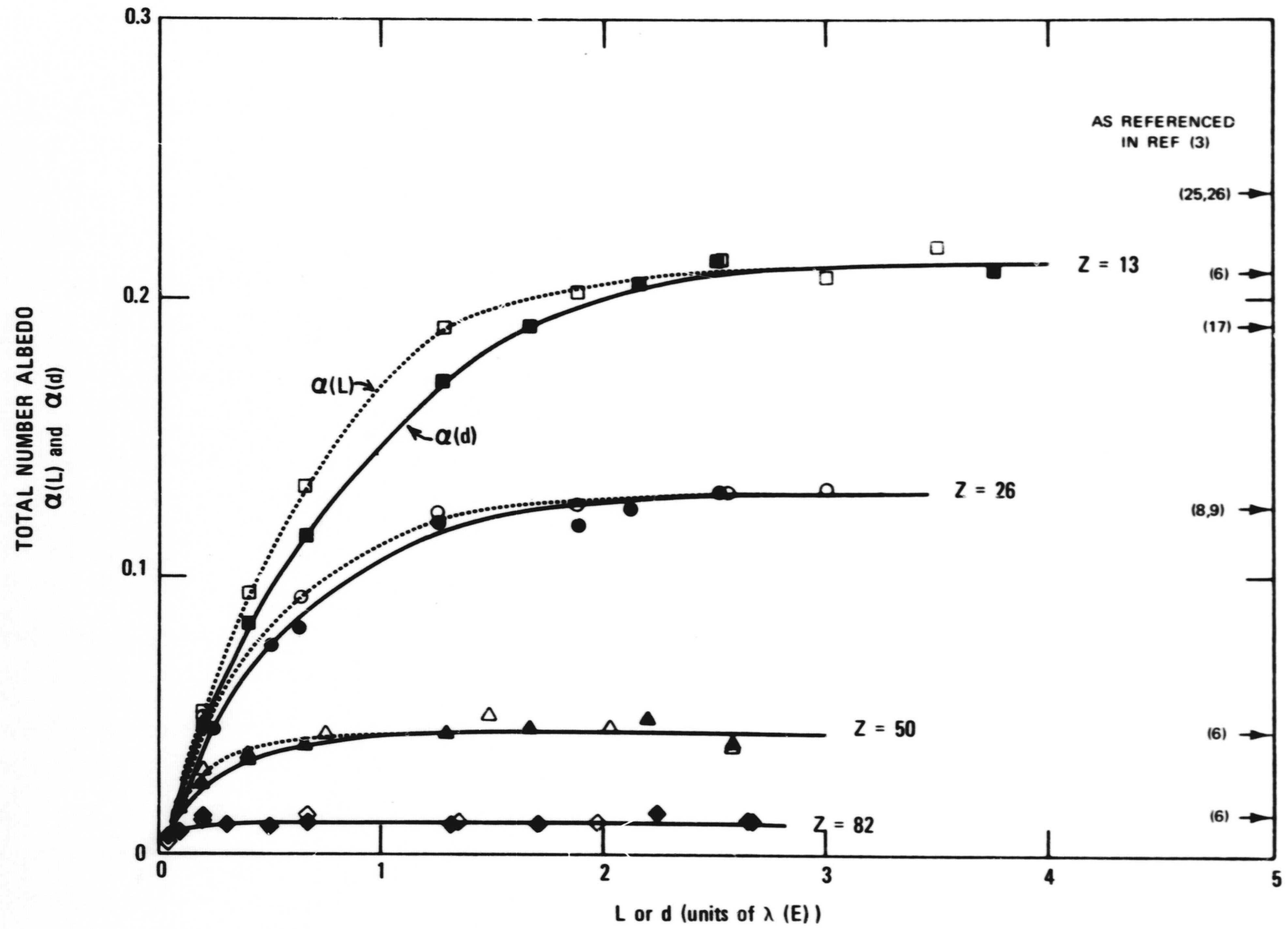
8. JAEGER, R. G., Editor-in Chief, "Engineering Compendium on Radiation Shielding", Vol. I: Shielding Fundamentals and Methods, 236-238, Springer-Verlag, New York, Inc. (1968).

9. MILLER, W. F. and SNOW, W. J., "NaI and CsI Efficiencies and Photofractions for Gamma-Ray Detection", Nucleonics, Vol. 19, N$\underline{o}$ 11, 174 (November 1961).

FIGURES

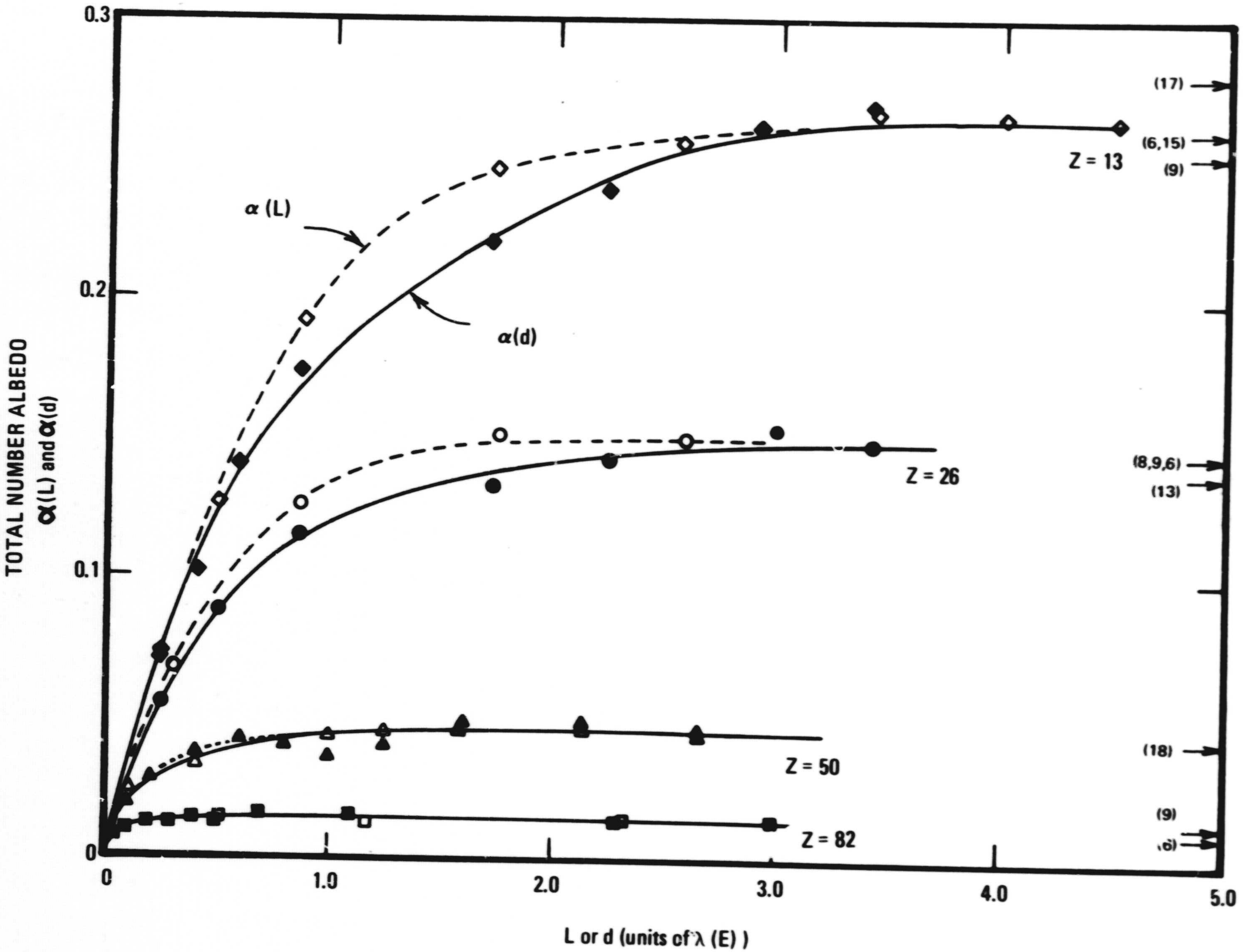


ALBEDO GEOMETRY
FIGURE 1

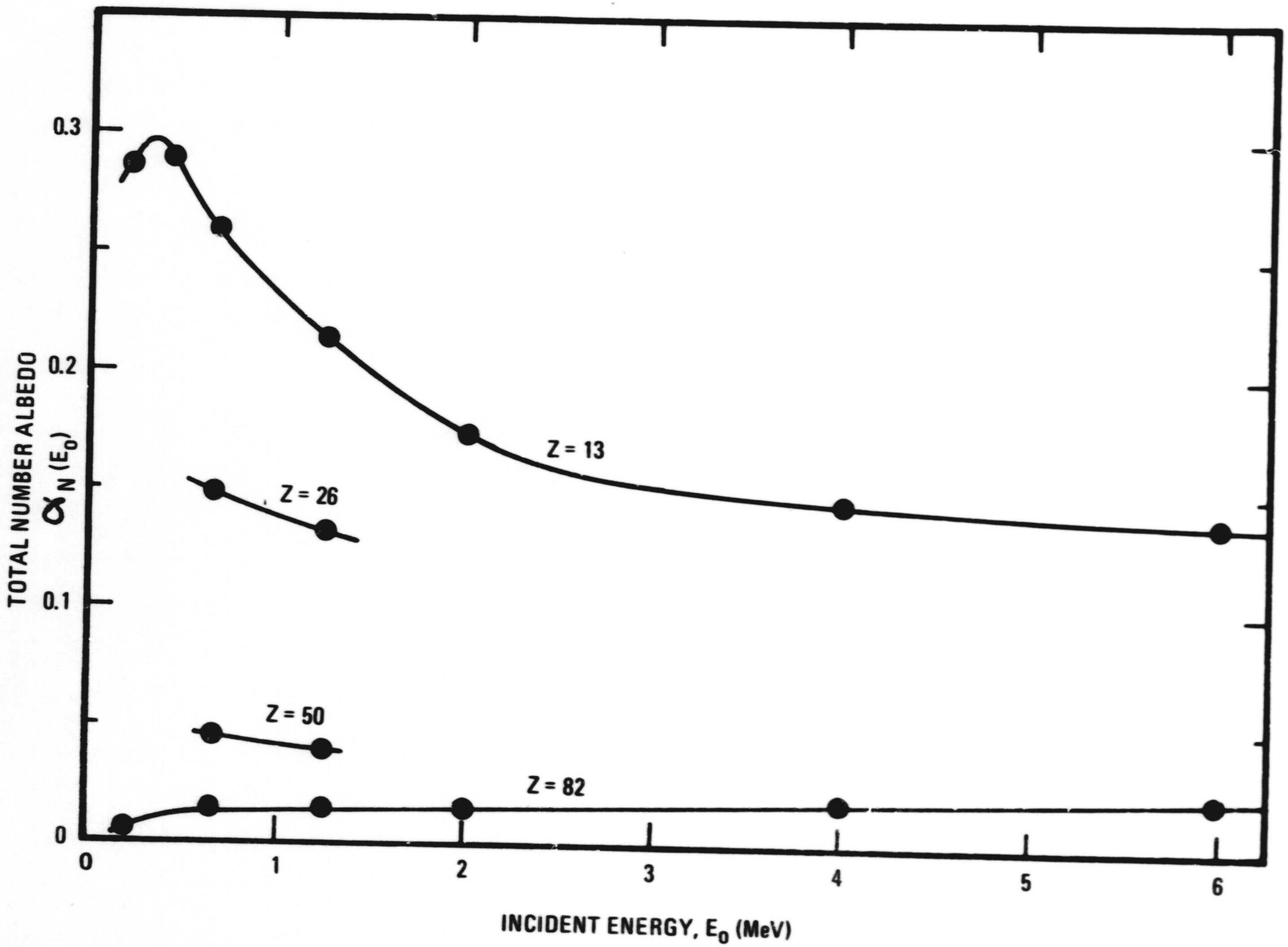


TOTAL NUMBER ALBEDO AS A
FUNCTION OF L and d FOR E = 1.25 MeV, and NORMAL INCIDENCE

FIGURE 2

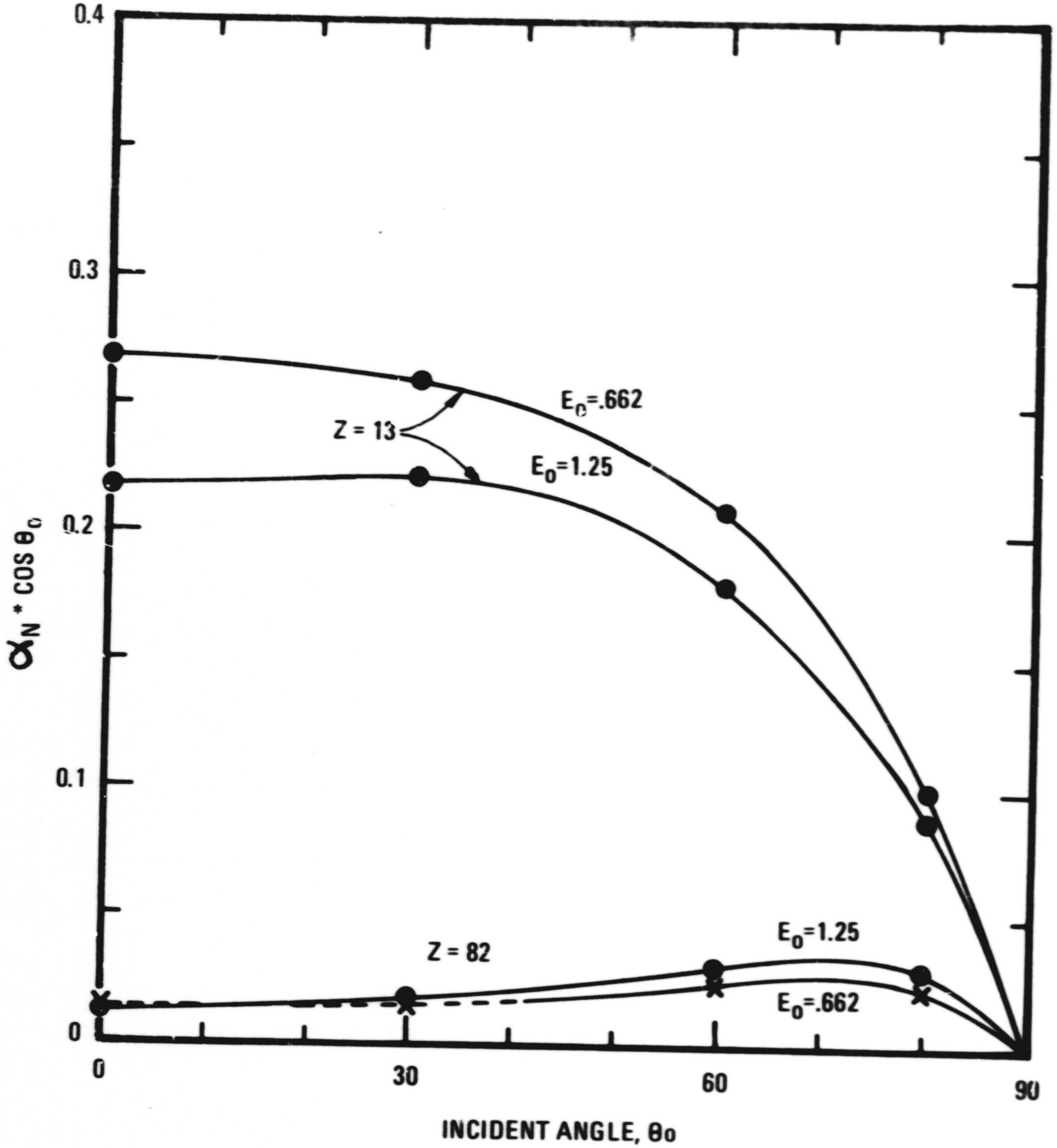


TOTAL NUMBER ALBEDO AS A FUNCTION OF L AND d
FOR E_o = 0.662 MeV AND NORMAL INCIDENCE
FIGURE 3



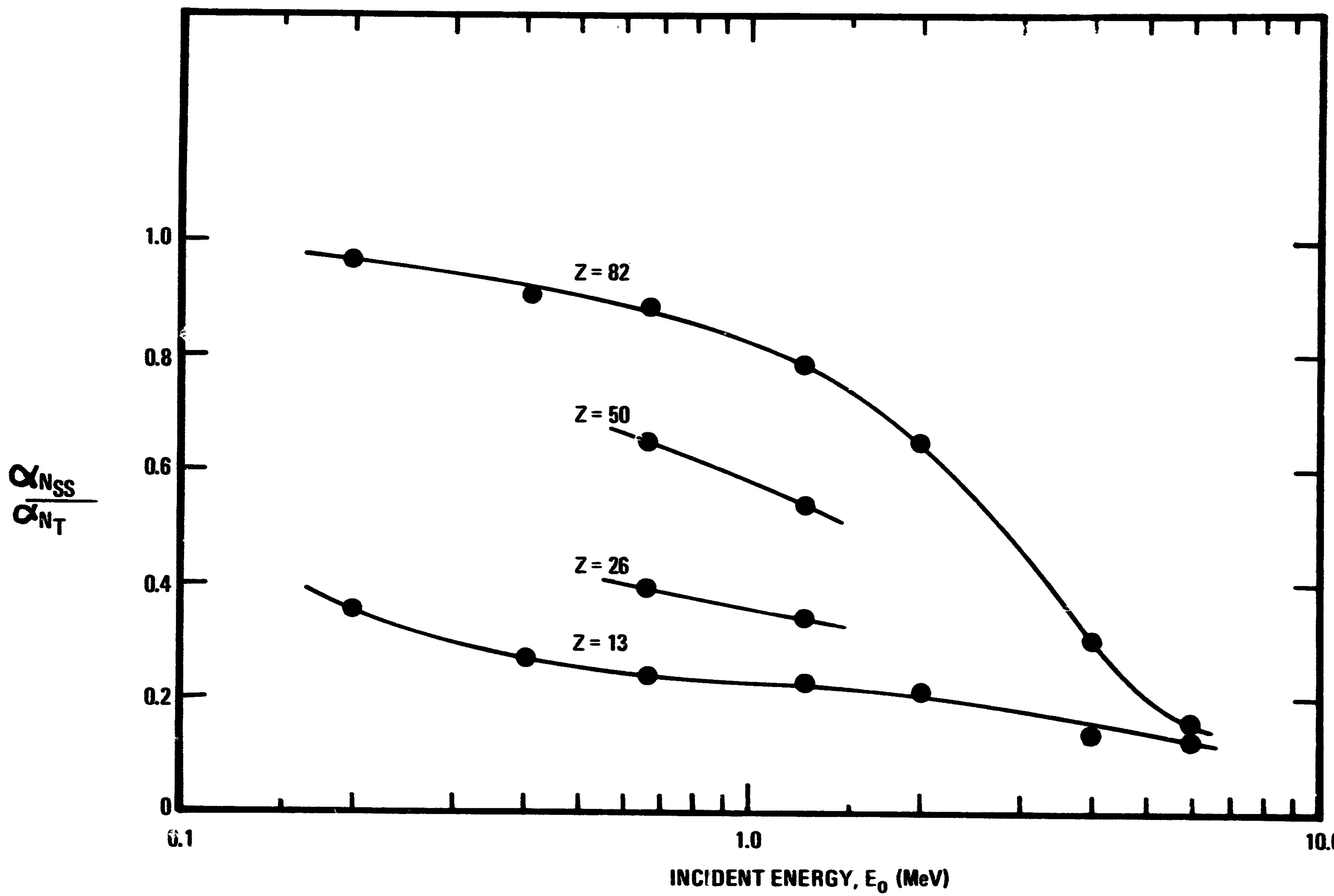
TOTAL NUMBER ALBEDO α_N AS A FUNCTION OF INCIDENT ENERGY E_o

FIGURE 4



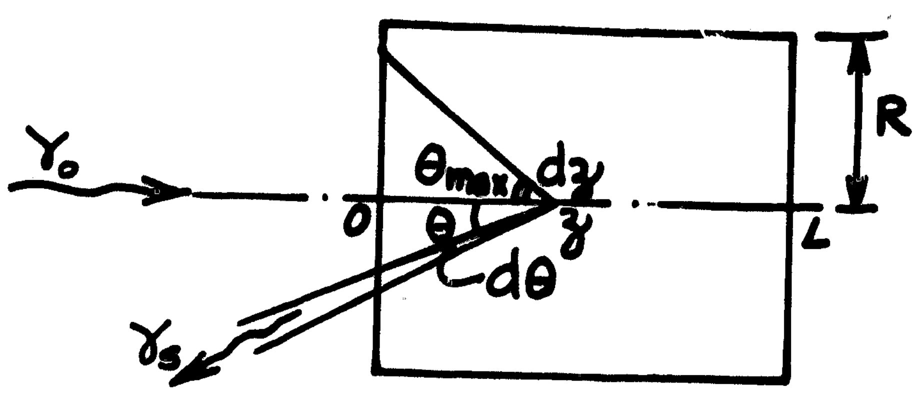
(TOTAL NUMBER ALBEDO α_N)* COS θ_o AS A FUNCTION OF INCIDENT ANGLE θ_o, FOR E_0=0.662 AND 1.25 MeV

FIGURE 5



SINGLE SCATTER/TOTAL NUMBER ALBEDO RATIO AS A FUNCTION OF INCIDENT ENERGY E_o

FIGURE 6



GEOMETRY FOR ANALYTIC
SINGLE BACKSCATTER EQUATION
FIGURE 7

TABLES

TABLE I

TYPICAL VALUES OF THE CHARACTERISTIC

DISTANCE $d_{1/2}$(IN UNITS OF λ (E))

ENERGY E (MeV)	ATOMIC NUMBER, Z			
	13	26	50	82
0.412	0.63	—	—	0.09
0.662	0.60	0.35	0.18	0.08
1.25	0.55	0.30	0.17	0.07

TABLE II

SINGLE AND DOUBLE SCATTER TOTAL NUMBER ALBEDO RATIOS

R_{ss}/R_{ds} ($R_{ss} = \alpha_{ss}/\alpha_T$ AND $R_{ds} = \alpha_{ds}/\alpha_T$)

ENERGY E (MeV)	ATOMIC NUMBER, Z			
	13	26	50	82
0.2	.36/.24	–	–	.965/.031
0.412	.27/.21	–	–	.90/.09
0.662	.24/.21	.39/.27	.65/.24	.88/.11
1.25	.22/.19	.34/.28	.58/.24	.79/.14
2.0	.21/.17	–	–	.65/.11
4.0	.14/.12	–	–	.30/.07
6.0	.13/.11	–	–	.15/.05

TABLE III

COMPARISON OF MONTE CARLO AND ANALYTIC SINGLE SCATTER TOTAL NUMBER ALBEDOS α_{SS}

MATERIAL	ENERGY (MeV)	d (cm)	L (cm)	$(\alpha_{SS})_{anal.}$	$(\alpha_{SS})_{mc}$
				X 10^{-2}	
Al	.622	17.0	17.0	6.56	6.42
			2.5	5.47	5.40
	1.25	17.0	17.0	4.71	4.79
			4.25	4.33	4.20
Fe	.662	6.0	6.0	4.29	4.48
			1.19	3.61	3.22
	1.25	6.0	6.0	5.82	5.77
			1.5	5.37	5.61
Sn	.662	5.0	5.0	2.92	2.89
			0.752	2.57	2.76
	1.25	7.0	7.0	2.48	2.13
			1.75	2.38	2.28
Pb	.662	4.0	4.0	1.12	1.30
			0.432	1.05	0.97
	1.25	4.0	4.0	1.02	1.06
			1.0	1.00	1.22