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PROGRAM BRAGG: A FORTRAN-IV PROGRAM FOR CALCULATING BRAGG CURVES, FLUX, AND CURRENT DISTRIBUTIONS, AND ENERGY SPECTRA

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Contents

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1. GENERAL DESCRIPTION

Program BRAGG is an extension of a program described earlier in a version[1] of this report. Some of the basic differences between the earlier and the current versions of BRAGG are inclusion of effects due to angular and energy distributions in the initial beam, and an option for inclusion of geometric attenuation of the beam as a result of beam spreading. BRAGG calculates Bragg, flux, and current curves for a beam of ions of arbitrary atomic number, atomic weight, and energy, incident on an absorber. This absorber is assumed to be homogeneous, but may consist of an arbitrary number of components, each specified by an atomic number, atomic weight, and atomic density. The geometry considered is that of a well-collimated beam incident on a slab whose transverse dimensions are large compared with the distance traveled in the absorber by the ions.

The calculation takes into account the processes of ionization energy loss, energy straggling, multiple scattering, and nuclear attenuation; energy deposition from secondary particles is neglected. The ionization energy loss and nuclear attenuation processes are calculated by means of distinct subroutines, which are intended for use either with protons or with ionized nuclei of heavy atoms. This flexibility has been deliberately incorporated, so that the user may easily employ his own routines for the calculation of these processes for any desired ion.

The initial beam either may be monoenergetic or may have a Gaussian energy distribution with an arbitrary standard deviation. Similarly, the initial beam either may be unidirectional (parallel to the normal of the slab face) or may have a Gaussian angular distribution with respect to the surface normal with an arbitrary standard deviation.

Various options for data output are available. The calculated curves may be printed in digital form, as on-line graphs, or as regular CalComp plots. The Bragg curves may be normalized to an arbitrary quantity, either at the origin or at the Bragg peak. Similarly, the flux and current curves may be arbitrarily normalized at the origin.

For graphic display purposes, an option permits shifting the calculated Bragg curve so that the Bragg peak is set at a specified depth of penetration.

The program also calculates the particle energy spectrum at the Bragg peak and at any other specified absorber depths. These may be printed out either in digital form or as CalComp plots.

Other options are available. Some of these pertain to control of the numerical procedure employed in the calculations, although the standard options that the program uses have been carefully chosen to yield the best results for most cases.

For comparison purposes, input data may be supplied to the program. These data are then plotted along with any CalComp figures output by the program.

Decks for Program BRAGG may be obtained from the Computer Center Library, Department of Mathematics and Computing, Lawrence Radiation Laboratory, Berkeley, California.

II. MATHEMATICAL MODEL

A detailed derivation and discussion of the equations upon which Program BRAGG is based is contained in Ref. 2. The purpose of this section is to outline briefly the basic mathematical expressions evaluated by BRAGG. All terms used are defined in Table I.

A. Particle Energy Spectrum

The spectrum at a given distance S is written as

$$M(E,S)dE = \frac{1}{\sqrt{\pi}} N_0(E_0)\exp\left\{-A_p\int_E^{E_0}[\Sigma(E')/f(E')]dE'\right\}\exp(-U^2)(dU/dE)dE, \quad (1)$$

which is defined as the number of particles at S having energies within an interval dE about E. The function U is defines as

$$U = \left[S - \bar{S}(E)\right] / \sqrt{2}\cdot\sigma(E,E_0) \quad (2)$$

and

$$\bar{S}(E) = A_p\int_E^{E_0}[1/f(E')]dE', \quad (2a)$$

where $\bar{S}(E)$ is the mean distance traveled by particles slowing down from energy E_0 to energy E.

The quantity $\sigma(E,E_0)$ is the standard deviation in the path-length distribution of particles with energy E, and it is equal to the square root of the variance of the path-length distribution. This variance is the sum of several terms, each of which represents the variance due to a particular effect. These effects include those due to angular and energy spreads in the initial beam, multiple scattering, and energy straggling.

Table I. Nomenclature

A_i	Atomic weight of the ith species of the target.
A_p	Atomic weight of beam ions.
C(S)	Total particle current at S, in charges/cm^2-sec.
CRIT1	Constant appearing in the equation describing validity of the δ-function approximation.
e	Electron charge in $(cm\text{-}MeV)^{1/2}$.
E	Energy of beam ions in MeV per Amu.
E_0	Initial energy of beam ions.
f(E)	Stopping power of ions of energy E, in MeV/(g/cm^2).
F(S)	Total flux at S, in particles/cm^2-sec.
FR	Step-size criterion parameter, used in numerical integration scheme.
$\hbar$	Planck's constant.
IADJ	Input parameter used in calculation of f(E).
D(S)	Total energy deposition rate per unit distance of travel at position S, in MeV/(g/cm^2)/sec.
MoC^2	Nucleon rest mass, 938 MeV.
M(E, S)dE	Number of ions per second with energies lying within an interval dE about energy E, at S.
$N_0(E_0)$	Initial number flux at target surface, in particles/cm^2-sec.
N_i	Atom density of the ith species of the target, in number/cm^3.
NT	Number of species in target.
R	Nuclear radius.
r_0, r_1	Reaction-cross-section parameters.
S	Distance of travel in the target, in g/cm^2.

$\bar{S}(E)$	Mean distance traveled by ions slowing down from energy E_0 to energy E.
SKT	Reaction-cross-section parameter.
$Z_{eff}(E)$	Effective charge of a particle of energy E.
Z_i	Atomic number of ith species of the target.
Z_p	Atomic number of beam ions.
ϵ	Total energy in the center-of-mass system.
$\eta_i(E)$	Microscopic total-reaction cross section for beam ions having energy E incident on the ith target species.
$\lambda(E)$	Wavelength of beam ions with energy E.
$\Sigma(E)$	Macroscopic total-reaction cross section for beam ions having energy E incident on the target.
$\sigma(E_0)$	Standard deviation in the range distribution of particles having initial energy E_0.
$\sigma(E, E_0)$	Standard deviation in the path-length distribution for particles slowed down from energy E_0 to energy E.

B. Number Density

The particle number density, also denoted as the number flux, or simply flux, is given at a particular distance S by

$$F(S) = \int_{\text{all } E} M(E, S)\, dE, \tag{3}$$

where M(E, S) is given by Eq. 1.

C. Dose

The relative dose at a distance S is given by

$$D(S) = \int_{\text{all } E} M(E, S) \cdot f(E)\, dE \tag{4}$$

D. Current

The total particle current at a given distance S is given by

$$C(S) = \int_{\text{all } E} M(E,S)\, Z_{\text{eff}}(E)\, dE, \qquad (5)$$

where $Z_{\text{eff}}(E)$ is the effective charge of a particle of energy E.

E. Cross Sections

The total microscopic cross section for the ith component of the target at a particular energy E is calculated from

$$\eta_i(E) = \pi \left[R_i + R_p + \lambda \right]^2 \left\{ 1 - \frac{Z_i Z_p E^2}{\epsilon \left[R_i + R_p + \lambda \right]} \right\} ; \qquad (6)$$

the ion wave length λ is given by

$$\lambda = (\hbar c / A_p) \left[2E(M_0 C^2) + E^2 \right]^{1/2}, \qquad (7)$$

and the c. m. energy is given by

$$\epsilon = \frac{A_i A_p}{A_i + A_p} E. \qquad (8)$$

The quantities R_i and R_p are the effective radii of the ion and the ith species of the target.[1] They are calculated by

$$R_k = \begin{cases} r_0 A^{1/3} + \text{SKT} & \text{for } A \geq 12 \\ r_1 A^{1/3} & \text{for } A < 12 \end{cases}, \qquad (9)$$

where R_k is either radius, and A is the corresponding atomic weight. In addition, special options are available for specifying the radius of either hydrogen or helium nuclei.

The total macroscopic cross section is given by the expression

$$\Sigma(E) = \sum_i \eta_i(E)\, N_i . \qquad (10)$$

F. Ionization Energy Loss

The function f(E) represents the stopping power of the ions due to ionization interactions with the atoms of the absorber. The calculation of this function is incorporated into a series of subroutines, and is based entirely on the work of Steward and Wallace.[3]

One important input parameter required for the calculation of f(E) is IADJ, which is related to the mean excitation energy for a particular absorber. The significance of this quantity is discussed by Barkas and Berger,[4] and a tabulation of values for all elements is given by Turner.[6]

III. INPUT FORMAT

The deck of input cards is subdivided into separate data decks (one for each problem) by blank cards. Each deck is arranged in the Random Input System, making input extremely easy and efficient.

A. Random Input System

The basic advantage of this system is that within a given data deck, the input cards may be arranged in any desired order, and one must supply only those cards necessary to the particular problem being run.

The deck consists of control cards and data cards. Data cards are seldom used, being necessary only when space on the associated control card is insufficient for the data being supplied by that control card. The first field on a control card indicates to the program which control card is being examined. In some cases, this field by itself specifies a particular option to be followed by the program. In other cases, the remaining fields supply data to the program. In a few cases, a control card indicates that a number of specific data cards immediately follow.

The format of all control cards is (A10, 3E10.0, 2A10). The first field contains an alphanumeric identifier, always left-justified. The remaining fields may or may not contain data, depending on the card. Table II gives a list of the control cards available as input to BRAGG. For several cards, the standard option is indicated in the table. This is the option chosen by the program in the absence of a control card specifying otherwise. In many cases, the standard option is the opposite of the control card specification and is not indicated in the table. For example, the PRINT DOSE control card specifies the printing of certain information. In the absence of this card, the information will not be printed.

A blank control card indicates the end of card input for that problem. Upon termination of a problem, the program reads in another data deck (the last card again being blank). The program terminates when an END control card is encountered.

Table II. BRAGG Control Cards

Columns 1 through 10	Function
BEAM**	(a) Beam atomic number and atomic weight, in fields 2 and 3.
	(b) Beam designation (alphanumeric identifier) in fields 5 and 6.
TARGET**	(a) No. of components in target (NT), target specific gravity, and value of IADJ in fields 2, 3, and 4.
	(b) Target designation (alphanumeric identifier) in fields 5 and 6.
	(c) Read (Z_J, N_J, A_J, J = 1, NT) from the next NT cards, in (3E10.0) format.
ENERGY**	Beam energy (MeV/amu) in field 2.
TITLE**	Read the 80-character title from the next card.
ENERGY SD**	Standard deviation in the initial energy distribution of the beam in field 2 (MeV/amu).
ANGULAR SD**	Standard deviation in the initial angular distribution of the beam in field 2.
BEAM DIAM**	Initial diameter of the beam (in centimeters) in field 2.
CRIT1**	Value of CRIT1 in field 2.
FR**	Value of FR in field 2.
NORM PDOSE**	Normalize the Bragg curve at the Bragg peak to the value in field 2.
NORM IDOSE**	Normalize the Bragg curve at the initial dose point to the value in field 2.
NORM FLUX**	Normalize the flux curve at the initial ordinate to the value in field 2.
NORM CURR**	Normalize the curve of current versus distance at the initial ordinate to the value in field 2.
PLOT DOSE	Plot the dose curve.
PLOT FLUX	Plot the flux curve.
PLOT CURR	Plot the curve of current versus distance.
STORE SPEC**	(a) Number of points (NSP) at which the spectra are to be saved internally for output (field 2).

	(b) Read NSP absorber depth values from the following cards in (8E10.0) format.
	(c) Calculate and store the spectra at the given depths.
PLOT SPEC	Plot the stored spectra.
DATA**	(a) NDT in field 2.
	(b) Read the NDT data points from the next NDT cards. The order of the data points is (YDATA;, XDATA;), in (2E10.0) format.
PLOT DATA	Plot the input data points along with the plotted curves.
NORM DATA**	Normalize the input data points so that the first point has the value in field 2.
PRINT DATA	Print out the input data points.
PRINT DOSE	Print the dose, flux, current, average energy, and average LET as a function of absorber depth.
PRINT SPEC	Print the stored spectra.
PRINT E	Print the energies used in calculating the various curves.
PRINT 2	Print the various energy-dependent quantities.
PRINT SCAT	Print the various quantities associated with the multiple-scattering process.
PLOT E	Plot the average energy as a function of absorber depth.
PLOT LET	Plot the average LET as a function of absorber depth.
SAME CURVE	Suppress all frame advancing (relative to plotting) for this problem.
PLOT GRID**	Plot grid lines with all figures.
RZERO**	Read the value of r_0 in field 2. (Standard option: 1.4)
RWUN**	Read the value of r_1 in field 2. (Standard option: 1.15)
SKIN T**	Read the value of SKT in field 2. (Standard option: -0.4)
X-ADJUST	Shift the calculated curves so that the Bragg peak is set at the absorber depth given in field 2.
R-H**	The value of RH is given in field 2. (Standard option: 0)
R-HE**	The value of RHE is given in field 2. (Standard option: 1.6)
CALL TABLE	Print a synopsis of the results of all problems executed since the last CALL TABLE card.
ONE FRAME	Advance the CalComp frame at the beginning of the problem (used with the SAME CURVE card).

X-AXIS SET**	Set the x-axis plotting parameters as follows:[6] (a) XMIN in field 2. (b) XMAX in field 3. (c) Number of intervals in the grid in field 4. (d) NXP in field 5.
Y-AXIS SET**	Set the Y-axis parameters as above.
QUICKPLOTD	Produce an on-line graph of the Bragg Curve.
QUICKPLOTN	Produce an on-line graph of the Flux Curve.
SAME CASE	The problem is the same as that preceding; skip the calculations but execute the current output options.
XDFACT	Multiply the input data abscissas by the value in field 2.
DATA2**	Same as the DATA control card, except that the order is (XDATA, YDATA).
TVPLOTS**	Plot all figures on the CRT CAMERA rather than the CalComp tape.

**See note 1 below.

B. Notes on Control-Card Use

1. In certain cases, once a particular option has been chosen, it will remain in effect for all the remaining problems in a job, or until another control card changes the option. The options for which this is true are indicated by a double asterisk in Table II. For example, insertion of the control card NORM PDOSE, with a 1.0 punched in the second field, will cause the calculated Bragg curves for each of the remaining problems to be normalized to unity at the peak.

Control cards not asterisked must be inserted in the data deck of each problem for which the corresponding option is to be exercised.

2. In using options for producing CalComp graphs, the following points should be remembered. A PLOT DATA control card will cause the program to plot the data points with each figure produced during the execution of a given problem. Therefore, it would normally be used when only one graph is to be plotted during a given problem. Similarly, the SAME CURVE control card prevents frame-advancing and axis-labeling during a given problem. It is normally used to plot several curves of the same type from successive problems on the same figure. Therefore, if either a PLOT DATA or SAME CURVE card is present in the data deck for a given problem, not more than one type of "plot" control card should be used in a given problem.

3. During execution, the standard printout consists of several key results, described in Section IV-A. These quantities are also written on the

file TAPE5 at the completion of each problem. Insertion of a CALL TABLE control card during a particular problem causes the following sequence: (i) After completion of the problem, TAPE5 is rewound: (ii) all results on TAPE 5 are printed on the standard output file in convenient tabular form; (iii) TAPE5 is rewound.

4. Regardless of the context, the quantities appearing in fields 2, 3, and 4 of any control card must have a decimal point or be right-justified within the field.

5. On the TARGET control card, NT is the number of components of the target; it is also equal to the number of data cards immediately following the TARGET card. Note that N_J is equal to the atom density times the factor 10^{-22}.

6. If the value of the standard deviation of the initial energy distribution is unspecified, it is taken to be zero. The same applies to the standard deviation of the initial angular distribution.

7. If a value for the initial beam diameter is specified, then attenuation factors due to beam spreading are applied. This option is applicable when the "detector" is assumed to have a very small sensitive area with respect to the cross-sectional area of the beam at all points.

If no value for the initial diameter is specified, then no geometric attenuation factors are applied.

IV. OUTPUT FORMAT

A. Standard Output

Various output options are available to the user by means of control cards. In all cases a certain amount of standard output is produced. This consists of a synopsis of the input data and a summary of key results. The first section includes the following:

1. Beam atomic number, atomic weight, and initial energy.

2. Target specific gravity and value of IADJ.

3. Atomic number, atomic weight, and atom density of each component of the target.

4. Values to be used by program for CRIT1, FR, r_0, r_1, and SKT. In addition, messages are printed indicating the modes to be used for flux and dose normalization and for axis shifting.

The second section of standard output contains the following:

1. The peak-to-initial-dose ratio.

2. The depth of penetration at the Bragg peak.

3. The average energy at the Bragg peak.

4. The mean range, defined as the penetration distance at which the dose has fallen to one-half that at the peak.

5. The percentage-detour factor, which is the percentage difference between the range and the corresponding mean distance of travel.

6. The mean beam deflection at the end of the range, equal to the mean distance of travel in a direction perpendicular to the initial direction of travel of the beam.

7. The fraction of the initial total energy accounted for. All energies are measured in units of MeV/amu, and all distances in units of g/cm^2.

B. Optional Output

The PRINT E card causes the program to print a list of the particle energies at which calculations are performed. The relationship between a given energy and the corresponding mean distance of travel is given by Eq. 2a.

The PRINT2 card causes the program to list, at each particle energy at which calculations are performed, the following quantities:

1. The energy.

2. The survival fraction, equal to the fraction of particles that have survived to that energy without undergoing a nuclear interaction.

3. The standard deviation in the range distribution at that energy.

4. The corresponding effective ion charge.

The PRINT DOSE control card causes the following quantities to be listed:

1. The penetration distance into the absorber.

2. The normalized or unnormalized dose.

3. The normalized or unnormalized flux.

4. The normalized or unnormalized current.

5. The average in energy.

6. The value of E, given by Eq. 2a.

7. The average LET.

The PRINT SCAT control card causes the printing of miscellaneous quantities associated with the calculation of the multiple-scattering correction, including:

1. The energy.

2. The actual mean distance of travel corresponding to that energy given by Eq. 2a.

3. The corresponding penetration distance.

4. The mean angle of deflection made by the particles with respect to the initial direction of travel.

5. The mean beam deflection, a quantity expressing the mean distance traveled by the particles in a direction perpendicular to the initial direction of travel.

6. The quantity THETAS, equal to the mean angle of deflection of the particles per unit length of travel. Its significance is discussed in Ref. 2.

The PRINT SPEC card produces a printout of the energy spectrum at the Bragg peak, calculated by use of Eq. 1. This spectrum is automatically normalized to 10.0 at the peak. It should be mentioned that the average energy at the peak is calculated by using this spectrum as a weighting function.

Use of the QUICKPLOTD and (or) QUICKPLOTN control cards will produce a plot of the dose and (or) flux curve on the standard output unit.

Several options may be exercised in the printing of CalComp plots. First, regular plots may be produced for any or all of the various calculated curves within a given problem by use of one or more of the corresponding control cards. In all cases, the axes are automatically labeled and numbered. Furthermore, a title is affixed to each figure produced. This is supplied by the TITLE control card. If a title is to be printed on a graph, it must not exceed 43 BCD characters. Any excess above this number will be lost. All plotted figures are sized to the standard 8.5×11-in. sheet.

The DATA, DATA2, and PLOT DATA control cards may be used to plot experimental data along with any of the calculated curves. The SAME CURVE control card may be used to overlay curves from different problems on the same figure (see Section III.C.2).

V. RESTRICTIONS

A. Mesh Size

The maximum allowable number of mesh points for a problem is 500. The total number of mesh points used depends on many variables, the chief ones being FR and CRIT1. The standard options used for these variables normally keep the number of mesh points well below 500. If different values are used, the number of points can in some cases exceed 500. If this occurs, an error message is printed, and the program goes on to the next problem.

B. Initial Energy

The maximum allowable initial energy is 1000 MeV/amu. This restriction is imposed by the routines that calculate f(E), and it can easily be modified.

C. Target Components

The maximum number of components of the target is set at 10.

D. Input-Data Points

The maximum number of data points that may be read in with a DATA or DATA2 control card is set at 300.

E. Title Card

The BCD characters on the card following the TITLE control card are printed on any CalComp plots produced, but no more than 43 characters are plotted. In all cases, the full 80 characters are printed along with the output.

APPENDIXES

A. Numerical Procedures

1. δ-Function Approximation

We consider the evaluation of the expression given by Eq. 4, and the associated expressions in Eqs. 1 and 2. For sufficiently small values of $\sigma(E, E_0)$, the term $(1/\sqrt{\pi})\exp\{-U^2\}\,[dU/dE]$ behaves like a δ function; and Eq. 4 reduces to

$$D(\bar{S}) = N_0(E_0)\exp\left\{-A_p\int_E^{E_0}[\Sigma(E')/f(E')]dE'\right\} f(E), \quad (11)$$

where $\bar{S}$ is given by Eq. 2a. We wish to learn when this approximation is valid. This may be deduced by the following argument. Consider the exponential term

$$T = \exp(-U^2), \quad (12)$$

where U is given by Eq. 2. For a given value of S, T is the controlling factor in determining how rapidly the total integrand in Eq. 4 goes to zero.

Thus, for $U \geq 3$, the contribution to the total integrand is negligible. Therefore, if each and every other factor in the integrand remains relatively constant over the energy interval within which the integrand differs significantly from zero, then the approximation of Eq. 4 by Eq. 11 is valid.

We state this mathematically as follows. Let D be the range covered by the variable S(E) over which the term T is significantly greater than zero. We may write

$$D = M\,\sigma(E, E_0), \tag{13}$$

where M is some constant in the neighborhood of 2 to 3. We wish to calculate the change in energy, ΔE, corresponding to the distance D. From Eq. 2a, we find that for a change in S(E) equal to D, the corresponding change in energy is approximately

$$\Delta E \approx \frac{D}{A_p}\, f(E) = M\,\sigma(E, E_0)\, f(E)\, \frac{1}{A_p} \quad . \tag{14}$$

We now require that the percentage change in each other factor in the integrand be less than some fraction h over the energy interval ΔE given by Eq. 14. The two functions to consider are

$$G_1(E) = \exp - \int_E^{E_0} A_p \quad [\,\Sigma(E')/f(E')\,]dE' \tag{15}$$

and

$$G_2(E) = f(E). \tag{15a}$$

For a given function $G_i(E)$, the percentage change over an increment ΔE is approximately

$$\frac{\Delta G_i}{G_i}(E) \approx \frac{dG_i(E)}{dE} \quad \frac{\Delta E}{G_i(E)} \quad . \tag{16}$$

Taking the derivatives of both functions in Eq. 15, using the approximation in Eq. 16 and the expression for ΔE in Eq. 14, and requiring that the percentage change of each function over ΔE be less than h, we obtain the criteria

$$\Sigma(E)\,\sigma(E, E_0) < \text{CRIT1} \tag{17}$$

and

$$\frac{dF(E)}{dE}\,\sigma(E, E_0) < A_p\,\text{CRIT1}, \tag{17a}$$

where

$$\text{CRIT1} = h/M\,. \tag{18}$$

If both of these requirements are satisfied for a reasonable value of h/M, then Eq. 4 may be replaced by the much simpler Eq. 11. Similarly, if Eq. 17 holds, then Eq. 3 may be replaced by

$$N(S) = N_0(E_0) \exp\left(- \int_E^{E_0} \frac{\Sigma(E')}{f(E')}\, dE'\right). \tag{19}$$

Experiment has shown that a value of CRIT1 equal to 0.01 produces excellent results. For larger values, the δ-function approximation begins to break down.

2. Numerical Integration

For those points at which the δ-function approximation is invalid, the integrals in Eqs. 3 and 4 are evaluated numerically, by use of the simple trapezoidal rule. In this case, the procedure is basically as follows:

1. Choose a set of energies $\{E_i\}$.
2. Calculate the set $\{\bar{S}_i\} = \{\bar{S}(E_i)\}$ for each energy by using Eq. 2a.
3. Evaluate the integral $A_p \int \Sigma(E')/f(E')dE'$ at each energy.

Finally, the numerical integration is performed for a set of values for the distance S. In fact, the evaluation is greatly simplified by choosing these values to coincide with the set $\{\bar{S}_i\}$.

It remains to choose the energy set $\{E_i\}$ at which the numerical calculations are to be performed. Since the term T given by Eq. 12 is the most rapidly varying in both Eqs. 3 and 4, we impose the requirement that in traversing the energy interval ΔE, which is the interval over which the trapezoidal rule is applied at any given step, the change in the quantity U be less than or equal to some fraction FR, where FR is a small fraction of unity. This ensures that the change in the exponential term T will likewise be small over the interval ΔE.

The change in U across ΔE is approximated by

$$\Delta U \approx \Delta\bar{S} \,/\sqrt{2}\, \sigma(E, E_0) , \tag{20}$$

where $\Delta \bar{S}$ is the difference between two successive members in the set $\{\bar{S}_i\}$.

It is assumed that $\sigma(E, E_0)$ remains relatively constant over the interval. We require, then, that

$$\Delta S/\sigma(E, E_0) \leq \sqrt{2}\ \text{FR}. \tag{21}$$

From Eq. 2a, the relation between the change in distance ΔS and the corresponding energy change ΔE is

$$\Delta E = \frac{1}{A_p}\ f(E)\,\Delta\bar{S} . \tag{22}$$

Substituting into Eq. 21, we obtain the restriction on ΔE:

$$\Delta E \leq \frac{1}{A_p}\ f(E)\,\sigma(E, E_0)\ \sqrt{2}\cdot \text{FR} . \tag{23}$$

Thus, for a given energy E_i, the next energy E_{i+1} at which the calculations

are performed is given by Eq. 23, where the equality sign is chosen. Therefore we can write

$$E_{i+1} = E_i - \Delta E. \tag{24}$$

Experimentally, it is found that a value for FR of approximately 0.2 is satisfactory.

B. Notes on Compatibility

Program BRAGG is written in Fortran-IV language for the Control Data Corporation 6600 computer system at the Lawrence Radiation Laboratory (LRL) in Berkeley, California. It can be used with a minimum of modification on practically any system that accepts Fortran-IV and that has adequate storage capacity. The chief alterations that might have to be made are outlined below.

1. Word Size

The CDC-6600 operates on a word size of 60 bits, or ten BCD characters. For machines using different word sizes, all instructions depending on the word size would have to be modified. These would be primarily the DATA statements appearing at the beginning of the main program; some of the WRITE or PRINT statements (and their associated FORMAT statements) that appear in the main program and in the subroutines GMPRINT and TABLE; and the series of logical IF statements appearing in the main program.

2. Graphing Routines

BRAGG contains the option of producing CalComp-drawn figures or CRT camera figures. The control statements for this process are contained in SUBROUTINE GMPRINT, and many of them refer to subroutines peculiar to LRL Berkeley. At other installations, these statements might have to be removed or replaced.

3. ENCODE and DECODE Statements

These statements occur in the subroutines FIXLBL, CENTER, and GMPRINT. The easiest method of eliminating these statements is by inserting a set of corresponding WRITE and READ statements to a scratch file.

4. CALL DATE Statement

This occurs in the beginning of the main program and in subroutine TABLE. DATE is an LRL routine which supplied the current date.

5. Input-Output Statements

The input and output statements may each take any of several forms; not all of these forms may be allowed on other systems.

C. Sample Problem

The input and output for a typical problem are given here. The case chosen is for 125-MeV protons in water. Only the standard printed output is selected, but CalComp plots are shown for all three calculated curves.

Figure 1 shows the input cards for the problem. The three pages preceding Fig. 1 show the standard output. Figures 2 and 3 show the CalComp plots of the Bragg curve and the flux curve.

This work was done under the auspices of the U. S. Atomic Energy Commission.

REFERENCES

1. G. M. Litton, Program BRAGG, A Fortran-IV Program for Calculating Bragg Curves and Flux Distributions, UCRL-17391, Feb. 1967.

2. G. M. Litton, Penetration of High-Energy Heavy Ions in Matter, with the Inclusion of Coulomb, Nuclear, and Other Stochastic Processes (Ph. D. Thesis), UCRL-17392, Aug. 1967.

3. P. G. Steward and R. W. Wallace, Calculation of Stopping Power and Range-Energy Values for any Heavy Ion in Nongaseous Media, UCRL-17314, Dec. 1966.

4. W. H. Barkas and M. J. Berger, Tables of Energy Losses and Ranges of Heavy Charged Particles, NAS-NRC 1133, 1964.

5. J. E. Turner, Values of I and IADJ . . . , NAS-NRC 1133, 1964.

6. B. Benson, J 6 BKY CC66 (CalComp program description).

02/20/68.

----------PROGRAM BRAGG----------

SAMPLE PROGRAM WITH PROGRAM BRAGG

----------INPUT DATA----------

BEAM PARTICLES	BEAM ATOMIC NUMBER	BEAM ATOMIC WEIGHT	BEAM INITIAL ENERGY (MEV/AMU)
PROTONS	1	1.00	125.00

STANDARD DEV. IN BEAM ENERGY (MEV/AMU)	STANDARD DEV. IN BEAM ANGLE (DEG.)	BEAM DIAMETER (CM)	R-ONE
1.0000E+00	0.	-	1.150

CRIT1	FR	SKT	RZERO
1.0000E-02	2.0000E-01	-.40	1.400

NO ADJUSTMENT OF THE ABSCISSAS HAS BEEN MADE

THE LET-DISTRIBUTION IS NORMALIZED TO 1.0000E+00 AT THE INITIAL ORDINATE

THE NUMBER-DENSITY DISTRIBUTION IS NORMALIZED TO 1.0000E+01 AT THE INITIAL ORDINATE

THE EFFECT OF BEAM SPREADING ON THE DOSE AND FLUX IS IGNORED.

----------TARGET DATA----------

MATERIAL DESIGNATION	SPECIFIC GRAVITY	IADJ
WATER	1.000	65.10

NUMBER OF COMPONENTS IN TARGET MATERIAL..... 2

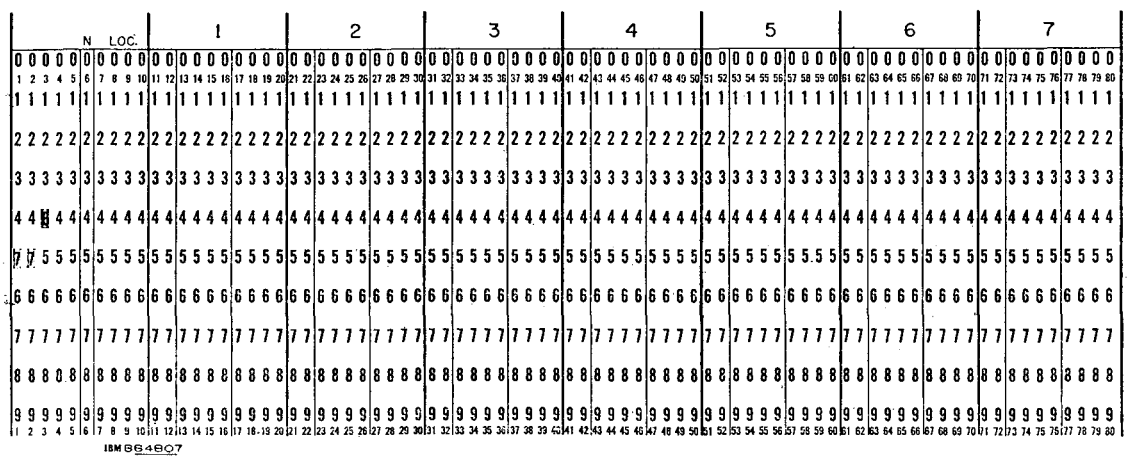
COMPONENT	ATOMIC NUMBER	ATOMIC WEIGHT	ATOM DENSITY (NC. PER CM**3)
1	8	16.000	3.3500E+22
2	1	1.000	6.6900E+22

SUMMARY OF RESULTS

SAMPLE PROGRAM WITH PROGRAM BRAGG

(BRAGG PEAK/INITIAL) DOSE RATIO.....	4.755E+00
PENETRATION DEPTH AT BRAGG PEAK (G/CM**2).....	11.0708
AVERAGE ENERGY AT BRAGG PEAK (MEV/AMU).....	14.7212
BRAGG PEAK FULL WIDTH AT HALF-MAXIMUM.....	1.197E+CO
MEAN RANGE (G/CM**2).....	11.3796
PERCENTAGE DETOUR FACTOR.....	.1065
MEAN BEAM DEFLECTION (G/CM**2).....	.3616
FRACTION OF ENERGY DEPOSITED BY PRIMARIES.....	.897

```
TITLE

SAMPLE PROBLEM WITH PROGRAM BRAGG

BEAM        1.0         1.0                    PROTONS

TARGET      2.0         1.0         65.1       WATER

8.0         3.35        16.0

1.0         6.69        1.0

ENERGY      125.0

ENERGY SD   1.0

PLOT FLUX

PLOT DOSE

NORM FLUX   10.0

NORM IDOSE  1.0


END
```



XBL683-1863

Fig. 1. Sample input.

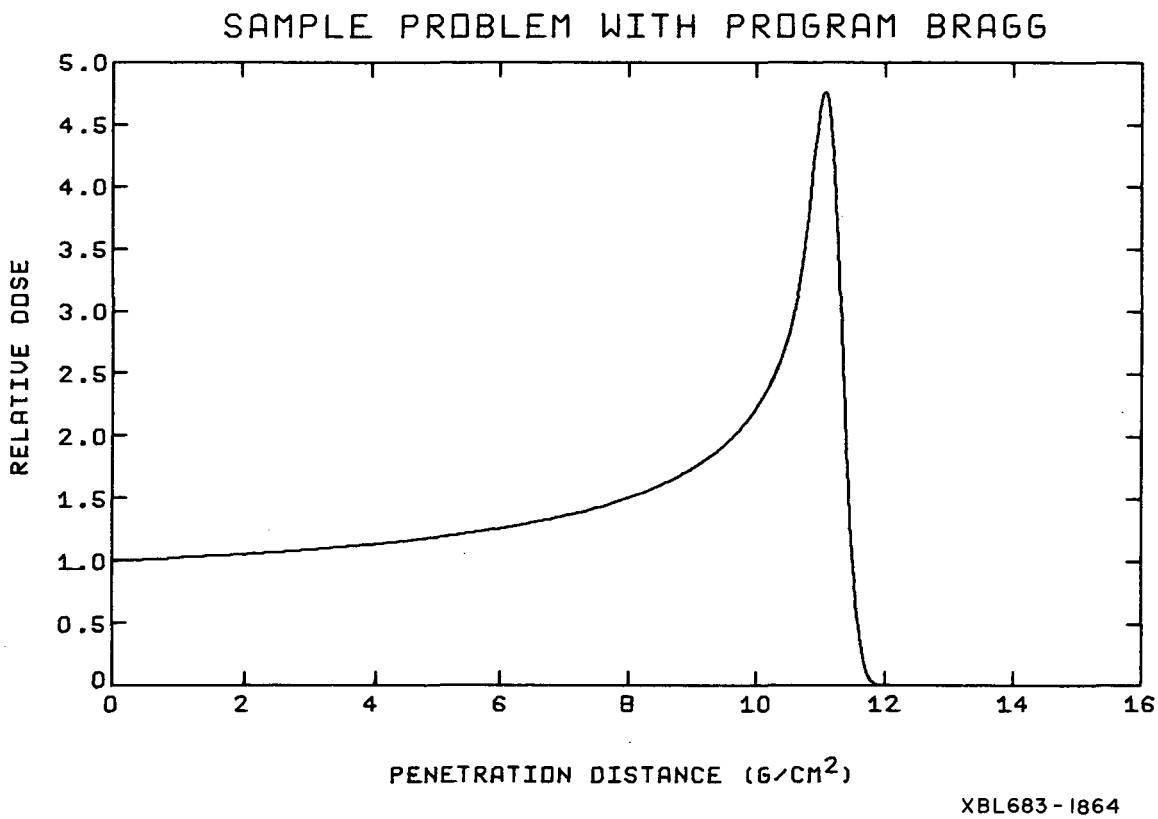


Fig. 2. Sample Bragg curve.

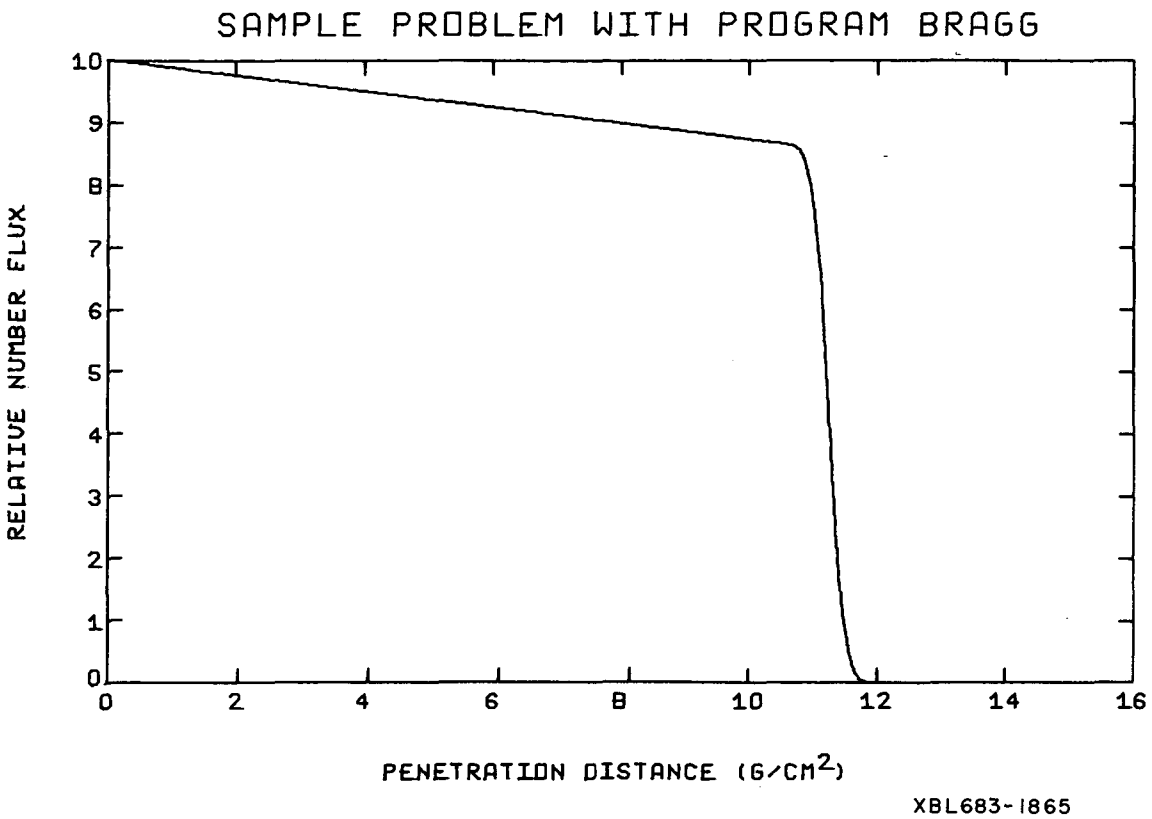


Fig. 3. Sample flux curve.