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**SPAR, A FORTRAN PROGRAM FOR
COMPUTING STOPPING POWERS AND
RANGES FOR MUONS, CHARGED PIONS,
PROTONS, AND HEAVY IONS**

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and Ranges for Muons, Charged Pions,
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*T. W. Armstrong
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**SPAR, a FORTRAN Program for Computing Stopping Powers
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T. W. Armstrong and K. C. Chandler

Abstract

SPAR is a FORTRAN IV program that computes the stopping powers and ranges for muons, pions, protons, and heavy ions in any nongaseous medium at energies from zero to several hundred GeV. The method of calculation and the input required are described, and computed stopping powers and ranges for various particles slowing down in water and in tissue are given.

I. INTRODUCTION

In studies related to the physical and biological effects produced by the penetration of charged particles through matter, numerical values for stopping powers and ranges are often needed for a variety of particle types and materials and over a large range of particle energies. The computer program described here was written to calculate stopping powers and ranges for muons, charged pions, protons, and heavy ions (mass number > 1) in any nongaseous medium at energies from zero to several hundred GeV.* Although guided in some instances by available experimental data, the method of calculation used is based predominantly on existing theories. The accuracy of the theoretical expressions used varies considerably over the wide range of variables considered, and in some cases (notably for very heavy ions at very low energies), generality in the program has been retained even though the results in some cases may be very approximate.

Stopping powers are computed using a different calculational procedure for each of three (β, z) regions, where β is the speed of the particle relative to the speed of light and z is the nuclear charge of the particle. At high energies ($\beta > 0.04 z^{2/3}$), where the particles can be considered to be completely ionized, Bethe's¹ theory with shell- and density-effect corrections is used. At intermediate energies ($0.0046 z^{1/3} < \beta \leq 0.04 z^{2/3}$), where charge reduction is important but energy losses from elastic Coulomb collisions can be ignored, an empirical expression² for the charge reduction

*SPAR is programmed to allow particle energies up to 1 TeV. However, the only energy-loss mechanisms taken into account at high energies are ionization and excitation. For the lighter particles, other energy-loss mechanisms become important for energies above several hundred GeV.

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is used in conjunction with Bethe's theory. At low energies ($0 \leq \beta \leq 0.0046 z^{1/3}$) where both charge reduction and nuclear Coulomb stopping are important, the theory of Lindhard *et al.*³ is used.

The stopping powers are computed using the continuous slowing-down approximation; i.e., fluctuations of the energy loss are disregarded. Thus, the stopping powers computed here correspond to the mean energy loss per unit path length due to collisions with electrons and, at very low energies, nuclear Coulomb scattering. The ranges are computed by numerical integration of the stopping powers. Therefore, the ranges computed here do not include the effects of energy-loss fluctuations (i.e., range straggling), multiple Coulomb scattering, or nuclear interactions (other than the energy loss in nuclear Coulomb scattering). For stopping media composed of compounds or mixtures, the stopping powers are computed assuming additivity of the stopping effects for each element.

The calculational method is described in Section II. In Section III some results computed using SPAR are shown and a few comparisons are made with available data. In Section IV some of the programming details of SPAR are discussed, and the input description is given.

II. METHOD OF CALCULATION

A. Stopping Powers

A different calculational procedure is used to compute the stopping powers in each of three (β, z) regions, where β is the speed of the particle relative to the speed of light and z is the nuclear charge of the particle.

Region I: $\beta > 0.04 z^{2/3}$

In this region, the gain and loss of electrons by the particle can be neglected, and the net charge of the particle is therefore the same as its nuclear charge. (For example, the boundary of this region, $\beta = 0.04 z^{2/3}$, corresponds to kinetic energies of about 0.75, 7.5, and 194 MeV for protons, alpha particles, and oxygen ions.) In this (β, z) region, the formula of Bethe with shell- and density-effect corrections (e.g., ref. 1) is used to compute the stopping power for protons, and the stopping powers for all other particles are scaled from the proton stopping power.

The stopping power for protons is computed from

$$S_p(E) = n \left[\frac{4\pi e^4}{m_e c^2} \right] \frac{z_p^2}{\beta^2} \left\{ \ln[2 m_e c^2 \beta^2 / (1 - \beta^2)] - \beta^2 - \ln \bar{I} - (\bar{C}/\bar{Z}) - \bar{\delta}/2 \right\},$$

where

$S_p(E)$ = the stopping power for protons at kinetic energy E ;

n = the electron density of stopping medium

$$= \sum_j N_j Z_j;$$

N_j = the atom density of j th type nuclide;

Z_j = the charge number of j th type nuclide;

e = the electronic charge;

$m_e c^2$ = the rest energy of an electron;

$\bar{I}$ = the ionization potential;

z_p^* = the effective charge of a proton (= 1 for $\beta > 0.04$);

$$\beta^2 = [(E/m_p c^2 + 1)^2 - 1]/(E/m_p c^2 + 1)^2 ;$$

$m_p c^2$ = the rest energy of a proton;

$(\bar{C}/\bar{Z})$ = the shell-effect correction;

$\bar{\delta}$ = the density-effect correction.

The quantities with bars indicate averages over all nuclide types in the stopping medium.

The average ionization potential is computed as

$$\ln \bar{I} = \frac{\sum_j N_j Z_j \ln I_j}{\sum_j N_j Z_j} .$$

The values used for I_j are given in Table I. For $Z \leq 13$, I_j values are from Barkas and Berger,⁴ Janni,⁵ and Sternheimer,⁶ and for $Z > 13$ the semi-empirical formula of Sternheimer⁶ is used.

For $E \geq 8$ MeV, the shell correction was computed using the equation given by Barkas and Berger⁴:

$$(\bar{C}/\bar{Z}) = (f_1 \bar{I}^2 + f_2 \bar{I}^3)/\bar{Z} ,$$

where

$$f_1 = a_1/\eta^2 + b_1/\eta^4 + c_1/\eta^5$$

$$f_2 = a_2/\eta^2 + b_2/\eta^4 + c_2/\eta^5$$

$$\eta^2 = (E/m_p c^2) (E/m_p c^2 + 2)$$

$$\bar{Z} = \sum_j N_j Z_j / \sum_j N_j$$

TABLE I
Ionization Potentials

Element	I (eV)
H	18.7
He	42.0
Li	39.0
Be	60.0
B	68.0
C	78.0
N	99.5
O	98.5
F	117.0
Ne	140.0
Na	150.0
Mg	157.0
Al	163.0

$Z > 13$

$$I = 9.76 Z + 58.8 Z^{-0.19}$$

$$a_1 = 0.422377 \times 10^{-6}$$

$$a_2 = 3.858019 \times 10^{-9}$$

$$b_1 = 0.0304043 \times 10^{-6}$$

$$b_2 = -0.1667989 \times 10^{-9}$$

$$c_1 = -0.00038106 \times 10^{-6}$$

$$c_2 = 0.00157955 \times 10^{-9}$$

The constants are for $\bar{I}$ in units of eV. For $E < 8$ the method of Lindhard and Sharff⁷ was used, where $(\bar{C}/\bar{Z})$ is expressed in terms of the dimensionless function $L(x)$ which is only weakly dependent upon the stopping medium.

$$(\bar{C}/\bar{Z}) = \ln \left[\frac{2m_e c^2 \beta^2}{\bar{I}} \right] - L(x)$$

where

$$x = (137)^2 \beta^2 / \bar{Z} .$$

Although $L(x)$ is only weakly dependent upon the stopping medium, it was found better to use values for $L(x)$ based on two different stopping media rather than to use the same $L(x)$ for all stopping media. Thus, $L_1(x)$ and $L_2(x)$ were determined for protons stopping in water and aluminum, respectively. For stopping media with $\bar{Z} \geq 13$, $L_2(x)$ was used; for $\bar{Z} \leq 3.33$, $L_1(x)$ was used; and for $3.33 < \bar{Z} < 13$, an interpolation in Z between $L_1(x)$ and $L_2(x)$ was made to obtain $L(x)$. $L_1(x)$ was determined by requiring the stopping power for water, computed using Eq. 1 and the above expression for $(\bar{C}/\bar{Z})$, to match the stopping power for protons in water given by the International Commission on Radiation Units and Measurements.⁸ Similarly, $L_2(x)$ was determined using the experimental stopping power for protons in aluminum at low energies given in Fig. 5 of the article by Northcliff.⁹ At high energies ($x > 24$), $L(x)$ values for aluminum were taken from the work of Turner as presented in Fig. 5 of the paper by Fano.¹ (These values for $L(x)$ were used both for $\beta \geq 0.04$ and for $\beta < 0.04$. When $\beta < 0.04$, the expression for z_p^* given later was used in Eq. 1.)

For the density-effect correction, an asymptotic form¹⁰ of the expression given by Sternheimer¹¹ is used at all energies:

$$\bar{\delta} = \ln(\alpha n \eta^2 / \bar{I}^2) - 1 ,$$

where

$$\alpha \equiv h^2 c^2 e^2 / \pi m_e c^2$$

h = Planck's constant.

When the above equation for $\bar{\delta}$ gives a negative value, $\bar{\delta}$ is set equal to zero.

Region II: $0.0046 z^{1/3} < \beta \leq 0.04 z^{2/3}$

For $\beta \leq 0.04 z^{2/3}$ the net charge of the particle becomes less than the nuclear charge because of electron capture.

For $\beta \geq 0.0046 z^{1/3}$ the energy loss due to elastic Coulomb collisions between the particle slowing down and the nuclei of the stopping medium, which is not taken into account by Eq. 1, is negligible. Therefore, in the (β, z) region defined by $0.0046 z^{1/3} < \beta \leq 0.04 z^{2/3}$, Eq. 1 is still applicable for protons but z_p^* is no longer unity. For the effective charge we use the empirical relation of Barkas,²

$$z_i^* = z_i [1 - \exp(-125 \beta z_i^{-2/3})] ,$$

and assume this relation to be valid for all particle types and all stopping media.

The stopping powers for other particles are obtained by scaling the proton stopping power:

$$S_i(E_i, z_i, m_i) = \frac{z_i^{*2}}{z_p^{*2}} S_p(E_i m_p / m_i) .$$

Region III: $0 \leq \delta \leq 0.0046 z_1^{1/3}$

In this region nuclear Coulomb stopping is important and stopping powers are computed using the theory of Lindhard et al.³

The electronic stopping power is computed as

$$S_1^e = k_1 \sqrt{E_1} ,$$

where k_1 is evaluated so that S_1^e and S_1 , calculated by the method used in Region II, have the same value at the boundary $\delta_1 = 0.0046 z_1^{1/3}$.

The theory of Lindhard et al. for the nuclear Coulomb stopping power uses the dimensionless parameters $dc/d\phi$ and c as measures of stopping power and energy, respectively. A universal curve relating $dc/d\phi$ and c for all particle types and stopping media is given by Lindhard et al. An analytic expression for this curve is given by Steward.¹² The relation between $dc/d\phi$ and c used here has the same functional form as Steward's expression but the constants have slightly different values.

The equations are:

$$\left(\frac{dc}{d\phi}\right)_{1j} = 4.51 \sqrt{c_{1j}} \exp(-2.54 c_{1j}^{0.277})$$

$$c_{1j} = F_j E_1$$

$$F_j = 3.255 \times 10^4 \frac{A_1 / (A_1 + m_1)}{z_1 z_j (z_1^{2/3} + z_j^{2/3})^{1/2}}$$

$$S_{1j}^n = \left(\frac{A_1 N_1}{N_a}\right) \left(\frac{dc}{d\phi}\right)_{1j} / G_{1j}$$

$$G_{1j} = 1.96 \times 10^{-4} \frac{A_1 (m_1 + A_1) (z_1^{2/3} + z_j^{2/3})^{1/2}}{z_1 z_j m_1} ,$$

where A_j , Z_j , and N_j are the mass, charge, and atom density, respectively, for the j th nuclide in the stopping medium, and N_a is Avogadro's number. The constants are for E_i in units of MeV and S_{ij}^n in units of MeV/cm.

The total stopping power for the medium is

$$S_i = S_i^e + \sum_j S_{ij}^n .$$

B. Ranges

For $E_i \leq E_{ci}$, where E_{ci} is the kinetic energy corresponding to $\beta_i = 0.04 z_i^{2/3}$, the range for all particle types is computed by numerical integration of the stopping power; i.e.,

$$R_i(E_i, z_i, m_i) = \int_0^{E_i} \frac{dE'_i}{S_i(E'_i, z_i, m_i)} .$$

For $E > E_{ci}$, the range for protons is computed by numerical integration of the proton stopping power, and the ranges for other particle types are scaled from the proton range; i.e.,

$$R_i(E_i, z_i, m_i) = R_i(E_{ci}, z_i, m_i) + \frac{(m_i/m_p)}{z_i^2} [R_p(E_i m_p/m_i) - R_p(E_{ci} m_p/m_i)] .$$

III. RESULTS

Although to date the SPAR code has not been tested extensively, the stopping powers and ranges computed by SPAR have been compared in a few cases with the work of others. The stopping powers of H, He, and O ions in Al have been compared with the stopping powers given by Northcliffe⁹ in the 0.01- to 10-MeV/amu range, and very good agreement is obtained. Figures 1, 2, and 3 show comparisons for the stopping powers of H, He, and O ions, respectively, in water. In Fig. 1, the stopping power of protons calculated here in the energy region from $\sim 10^{-3}$ to 8 MeV necessarily agrees with the ICRU stopping powers⁸ because the shell-correction term for the electronic stopping power was chosen to match the ICRU stopping powers in this energy region. The stopping powers shown in Figs. 1 and 2 from Steward¹² for energies < 10 MeV/amu were computed using smoothed stopping-power curves for various ions in aluminum from Northcliffe,⁹ together with relative stopping powers from several sources. Above 10 MeV/amu, Steward used Bethe's formula. The stopping powers from Northcliffe and Schilling¹³ were also generated using a set of master cross-section curves for aluminum in conjunction with relative stopping powers. The stopping powers shown in Figs. 2 and 3 from Caswell and Berger¹⁴ were obtained by using the theory of Lindhard *et al.*³ for the nuclear stopping power to extend the stopping powers of Northcliffe and Schilling¹³ (which include only electronic stopping) to lower energies. Thus, in Figs. 2 and 3 the stopping powers of Caswell and Berger¹⁴ and those of Northcliffe and Schilling¹³ necessarily coincide at those energies where nuclear stopping is negligible. The stopping powers for alpha particles from Tisljar-Lentulis *et al.*¹⁵ are based on measurements and calculations from several sources. Figure 4 shows a

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Fig. 1. Proton stopping power in water. The stopping power computed by SPAR is compared with those given by the International Committee on Radiation Units and Measurements (ICRU),⁸ Northcliffe and Schilling,¹³ and Steward.¹²

Fig. 2. Alpha-particle stopping power in water computed by SPAR and as given by Northcliffe and Schilling,¹³ Steward,¹² Caswell and Berger,¹⁴ and Tisljar-Lentulis *et al.*¹⁵

Fig. 3. Stopping power for oxygen ions in water computed by SPAR and as given by Northcliffe and Schilling¹³ and Caswell and Berger.¹⁴

Fig. 4. Ranges for protons, alpha particles, and oxygen ions in water. Also shown are ranges given by the ICRU⁸ and by Northcliffe and Schilling.¹³

comparison of ranges for protons, alpha particles, and oxygen ions in water.

As further examples of SPAR output, Figs. 5-8 show stopping powers and ranges for various ions in tissue ($\bar{\rho} = 1.0 \text{ g/cm}^3$). The following concentrations were used for tissue (in atom %): H, 63.3; O, 25.8; C, 9.5; and N, 1.4.

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Fig. 5. Stopping powers in tissue for muons (μ), pions (π), protons (p), deuterons (d), tritons (t), ${}^3\text{He}$ ions (${}^3\text{He}$), and alpha particles (α).

Fig. 6. Stopping powers in tissue for lithium (Li), beryllium (Be), boron (B), carbon (C), nitrogen (N), and oxygen (O) ions.

Fig. 7. Ranges in tissue for muons (μ), pions (π), protons (p), deuterons (d), tritons (t), ^3He ions (^3He), and alpha particles (α).

Fig. 8. Ranges in tissue for lithium (Li), beryllium (Be), boron (B), carbon (C), nitrogen (N), and oxygen (O) ions.

IV. THE SPAR PROGRAM

Description of Principal Subroutines

The SPAR program, written in FORTRAN IV, consists basically of subroutines PREP, DEDX, and RANGE, and a main program for calling these subroutines with the energies, particle types, and media for which stopping powers and ranges are desired. Since there may be occasions where it is desired to incorporate these main subroutines and auxiliary subroutines into other programs rather than use the standard main program, brief descriptions of PREP, DEDX, and RANGE are given below.

Subroutine PREP, which has no calling arguments, is called once by the main program to read in most of the input. The input description is given later.

Subroutine DEDX computes the stopping power and has the following arguments:

```
CALL DEDX(ITYP,XM,Z,EI,MED,STPI)
```

where

ITYP = particle type

= 1, heavy ion (i.e., mass number > 1)

= 2, proton

= 3, pion

= 4, muon

XM = mass of particle in amu. XM for protons, pion, and

muons is set internally in DEDX. Therefore, XM is

irrelevant in the calling argument except when ITYP = 1.

Z = charge number

EI = energy in MeV at which stopping power desired

MED = medium number. MED is defined by the order in which
the material composition is read in - see input description.

STPI = stopping power in MeV/cm at energy EI for a particle of
mass XM and charge Z in medium MED.

Subroutine RANGE computes the range and has the following arguments:

CALL RANGE(ITYP,XM,Z,EI,MED,RNGI)

where RNGI is the range in cm and all other arguments are the same as defined above.

In the case of computing ranges for heavy ions ($A > 1$), the first time that RANGE is called for a particular ion and material the range at various energies from zero to the energy corresponding to $\beta = 0.04 z^{2/3}$ is computed and stored, and the range at energy EI is returned. (For energies higher than that corresponding to $\beta = 0.04 z^{2/3}$, the heavy-ion range is scaled from the proton range.) Upon subsequent calls to RANGE for this same type of ion and material, the range at energy EI is interpolated from the stored ranges. In the standard version of SPAR, range vs energy for various ion types and materials is computed by calling RANGE inside DØ loops on ion type, material, and energy with energy varying most rapidly. Thus, present dimensions allow ranges to be stored in RANGE for only one type of ion and material at any one time. In applications where RANGE is to be called with ion type, material, and energy unordered, the computation time can be lessened by increasing certain dimensions in RANGE to allow ranges for more than one ion to be stored at the same time. Ranges in RANGE are stored in the array called RNGI with dimensions RNGI(125,1). To store the ranges for N different ion types and M different materials at one time, the dimension 1

for arrays RNGI(125,1), ZA(1), XMA(1), MEDA(1), ECUT(1), RECUT(1), PRECUT(1), and EINC2(1) should be changed to M*N. In addition, the variable IMAX, initialized in a data statement in subroutine RANGE, should have the value M*N.

Input Description

Card A: ^aFORMAT (I5)

- a. **MXMAT**: The number of different media for which stopping powers and ranges are to be computed ($0 < \text{MXMAT} \leq 15$).

The following cards, B_M and $C_{M,1}, \dots, C_{M,\text{NEL}(M)}$ are input for each medium:

Card B_M : ^a^b^cFORMAT (i5,F10.3,F10.3)

- a. **NEL(M)**: The number of nuclide types other than hydrogen in medium M ($1 \leq \text{NEL}(M) \leq 10$).
- b. **DENH(M)**: The density (atoms/cm³) of hydrogen in medium M multiplied by 10^{-24} .
- c. **AVDEN(M)**: The average density (g/cm³) of medium M.

Card(s) $C_{M,N}$: ^a^b^cFORMAT (F10.3,F10.3,F10.3)

- a. **ZZ(N,M)**: The charge number of the Nth nuclide in the Mth medium.
- b. **A(L,M)**: The mass number of the Nth nuclide in the Mth medium.
- c. **DEN(L,M)**: The atom density (atoms/cm³) of the Nth nuclide other than hydrogen in the Mth medium multiplied by 10^{-24} .

The order of the B_M and $C_{M,N}$ cards is: $B_1, C_{1,1}, C_{1,2}, \dots, C_{1,\text{NEL}(1)}, B_2, C_{2,1}, C_{2,2}, \dots, C_{2,\text{NEL}(2)}, \dots, B_{\text{MXMAT}}, C_{\text{MXMAT},1}, C_{\text{MXMAT},2}, \dots, C_{\text{MXMAT},\text{NEL}(\text{MXMAT})}$.

The medium number, **MED**, which is used internally in designating each medium, is determined by the order in which the medium information is read in. **MED** corresponds to the index **M** used in describing cards **B** and **C**.

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Card D: FORMAT (F10.^a3,F10.^b3)

- a. EMIN: Minimum energy in MeV for which stopping powers and ranges desired ($EMIN \geq 0.$).
- b. EMAX: Maximum energy in MeV for which stopping powers and ranges desired ($EMIN < EMAX \leq 1 \times 10^6$ MeV).

Card E: FORMAT (I^a5)

- a. NPTS: The stopping powers and ranges will be computed at NPTS energies spaced logarithmically between EMIN and EMAX.

Card(s) F: FORMAT (I^a5,F10.^b3,F10.^c3)

- a. ITYP: Denotes type of particle for which stopping powers and ranges are to be calculated.

ITYP = 1 for heavy ions (i.e., mass number > 1)

= 2 for protons

= 3 for pions

= 4 for muons

- b. Z: Charge number of ion. Z is irrelevant if ITYP $\neq$ 1.

- c. A: Mass (in amu) of ion. A is irrelevant if ITYP $\neq$ 1.

Card G: Blank Card

One F card is required for each type of particle for which stopping powers and ranges are to be computed. There is no restriction on the order or the number of F cards used.

Cards A through C are read by subroutine PREP and cards D through G are read by the main program.

Output

The printed output from SPAR consists of the input read by PREP followed by a table of stopping powers and ranges at various energy points for each type of particle and stopping medium. Each table contains (a) energies, in MeV/amu; (b) energies, in MeV; (c) stopping powers, in MeV/cm; (d) stopping powers divided by the square of the charge of the particle, in MeV/(mg/cm²); (e) ranges, in cm,; and (f) ranges, in mg/cm².

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