MASTER

**OAK RIDGE NATIONAL LABORATORY**

operated by

**UNION CARBIDE CORPORATION**

for the

**U.S. ATOMIC ENERGY COMMISSION**

**ORNL-TM-196**

COPY NO. - 1

DATE - April 11, 1962

# EVAP - A FORTRAN Program for Calculating the Evaporation of Various Particles from Excited Compound Nuclei

Lawrence Dresner



1a

## 1. Introduction

Nuclear bombardment by sufficiently energetic particles, such as the protons of the inner Van Allen belt or those originating in solar flares, usually produces excited compound nuclei after an intranuclear cascade. These compound nuclei are capable of de-exciting by the emission of various particles, e.g., neutrons, protons, deuterons, etc. The emitted neutrons form a very penetrating component of the radiation against which the crew of any prospective space vehicle must be shielded. In order to analyze the shielding requirements for space vehicles, it is consequently necessary to be able to calculate among other things the number of neutrons emitted from any compound nucleus and their energy spectrum. The FORTRAN program described in this report has been written for this purpose. This report is arranged as follows: In Section 2 the theory of the calculation is briefly described, in Section 3 the method of computation is explained, and in Section 4 operating instructions are given.

## 2. Theory

2.1. The theory of the emission of particles from excited compound nuclei is originally due to Weisskopf.[1] An excellent review of Weisskopf's theory and its developments up to 1958 has been written by LeCouteur.[2] Recently Dostrovsky *et al.*[3] have described a Monte Carlo code based on this theory; the program described in this memo is essentially the same one. A few changes have been made, however, and for the sake of completeness the formulae used in the computation are listed below together with some comments.

2.2. According to Weisskopf the probability $p(\epsilon)$ that an excited nucleus will emit a particle x with kinetic energy $\epsilon$ is proportional to

$$(2S_x + 1) \;\; m_x \;\; \epsilon \, \sigma_{cx}(\epsilon) \;\; \omega(E) \tag{1}$$

where

$S_x$ = the spin of particle x,

$m_x$ = the mass of particle x,

$\sigma_{cx}$ = the cross section for formation of the compound nucleus in the inverse reaction, i. e., by bombarding the residual nucleus with x's of energy $\epsilon$,

$E$ = the excitation of the <u>residual</u> nucleus and is less than the excitation of the compound nucleus by the sum of the binding and kinetic energies of x, and

$\omega(E)$ = the density of levels of the residual nucleus at excitation E.

2.3. The form of $\omega(E)$ is that given by Blatt and Weisskopf,[4] namely,

$$\omega(E) \;=\; \omega_o \exp\left(2\sqrt{a(E-\delta)}\right) \tag{2}$$

where a and $\omega_o$ are constants for a given nucleus and $\delta$ is the pairing energy. $\omega_o$ is considered to be a slowly varying function of mass and charge number (A and Z); since only ratios of expressions like (1) enter the calculation, its value is immaterial. According to LeCouteur,[2]

$$a = \frac{A}{B}\left(1 + Y\ \frac{\Delta^2}{A^2}\right) \tag{3}$$

where

$A$ = mass number,

$\Delta$ = $A - 2Z$,

$Z$ = charge number, and

$B, Y$ = universal constants.

LeCouteur's analysis indicates $Y \approx 1.5$; other work of Lang and LeCouteur[5] suggests $B \sim 8$ Mev.

The pairing energies, $\delta$, have been tabulated by Cameron[6] and his values are used in this work.

2.4. The inverse cross sections $\sigma_{cx}(\epsilon)$ used in this work are those recommended by Dostrovsky _et al_. For neutrons

$$\sigma_{cn}(\epsilon) = \alpha(1 + \beta/\epsilon)\ \pi R^2 \tag{4a}$$

$$\alpha = 0.76 + 1.93\ A^{-1/3} \tag{4b}$$

$$\alpha\beta = 1.66\ A^{-2/3} - 0.050 \tag{4c}$$

$$R = 1.70 \times 10^{-13} \text{ cm} \times A^{1/3} \tag{4d}$$

For charged particles

$$\sigma_{cx}(\epsilon) = (1 + C_x)(1 - k_x V_x/\epsilon) \pi R^2 \qquad \epsilon \geq k_x V_x \tag{5}$$

$$= 0 \qquad \epsilon < k_x V_x$$

where the constants $C_x$ and $k_x$ are given as follows:

| Z | $k_p$ | $C_p$ | $k_\alpha$ |
|---|---|---|---|
| 10 | 0.36 | 0.08 | 0.77 |
| 20 | 0.51 | 0.00 | 0.81 |
| 30 | 0.60 | -0.06 | 0.85 |
| 40 | 0.66 | -0.10 | 0.89 |
| 50 | 0.68 | -0.10 | 0.93 |
| 60 | 0.69 | -0.10 | 0.97 |
| ≥70 | 0.69 | -0.10 | 1.00 |

$$C_d = (1/2)\, C_p; \qquad C_{H^3} = (1/3)\, C_p; \qquad C_x = 0,\ Z \geq 2 \tag{6a}$$

$$k_d = k_p + 0.06; \qquad k_{H^3} = k_p + 0.12; \qquad k_{He^3} = k_\alpha - 0.06 \tag{6b}$$

$$k_x = 1.00,\ A > 4$$

The Coulomb barrier $V_x$ is given by

$$V_x = \frac{Z_x Ze^2}{R + R_x} \tag{7}$$

where $Z_x$ is the charge number of x, e is the charge of the proton, and

$R_x$ is given by the table

| A | $R_x$ |
|---|---|
| $2 \leq A \leq 4$ | $1.20 \times 10^{-13}$ cm |
| 6 | 2.02 |
| 7 | 2.43 |
| 8 | 2.84 |
| 9 | 3.25 |
| $\geq 10$ | $1.70A^{1/3}$ |

2.5. The determination of binding energies is done using the masses tabulated by Wapstra[7] and Huizenga[8] for nuclei for which the mass has been measured and the masses calculated with the semi-empirical formula of Cameron[9] for nuclei for which there are no measurements. To allow for easy inclusion of additional or improved mass data, the measured masses are treated as input data rather than as an integral part of the program. More will be said about this point later.

2.6. The following particles may be emitted from any compound nucleus: neutrons, protons, deuterons, tritons, $He^3$, alpha particles, $He^6$, $Li^6$, $Li^7$, $Be^7$, $Li^8$, $Li^9$, $Be^9$, and $Be^{10}$. $Li^6$, $Li^7$, $Be^7$, $Li^8$, and $Be^{10}$ have excited states lying, respectively, 3.56, 0.477, 0.430, 0.970, and 3.37 Mev above the ground state, and these states are treated as distinct particles for the purpose of this computation.

## 3. Method of Computation

3.1. The Monte Carlo method of computation is used. The starting point of a history is given by three numbers A, Z, and U, which serve to identify the compound nucleus and give its initial excitation. The first thing which is done is the computation of the total probability of emission of each of the 19 different kinds of particles which are considered by the code. This is done by calculating the quantities*

$$R_x = (2S_x + 1)\, m_x \int_{k_x V_x}^{U-Q_x-\delta} \epsilon\sigma_{cx}(\epsilon)\ \omega(U-Q_x-\delta-\epsilon)\, d\epsilon \qquad (8)$$

where $Q_x$ is the binding energy of x in the compound nucleus.

Dostrovsky et al., have pointed out that these energy integrals can all be done analytically. The $R_x$ are given by the following formulae:

$$R_x = A^{2/3}\ \alpha\, [I_1(S) + \beta\, I_o(S)]\, e^S \quad \text{(neutrons)} \qquad (9a)$$

$$R_x = \tfrac{1}{2}(2S_x + 1)\, m_x\, (1 + C_x)\, A^{2/3}\ I_1(S)\ e^S \text{(charged particles)} \qquad (9b)$$

$$S = 2\sqrt{a(U - k_xV_x - Q_x - \delta)} \qquad (k_x = 0 \text{ for neutrons}) \qquad (9c)$$

$$I_o(S) = (2a)^{-1}\, (S - 1 + e^{-S}) \qquad (9d)$$

$$I_1(S) = (8a^2)^{-1}\, (2S^2 - 6S + 6 + e^{-S}\, [S^2 - 6]) \qquad (9e)$$

where A, $\alpha$, $\beta$, a, $\delta$, k, V all refer to the residual nucleus. Eq. 9 is used only if $U \geq k_xV_x + Q_x + \delta$; otherwise $R_x$ is set equal to zero.

---

*The appearance of the pairing energy, $\delta$, in the upper limit of the integral is discussed by Dostrovsky et al. In passing from (8) to (9) the $R_x$ have been divided by a common numerical factor.

3.2. Next $\sum_{x=1}^{19} R_x$ is calculated. If it is zero, the history is terminated; otherwise the total emission probabilities are calculated according to the formula

$$P_x = R_x / \left( \sum_{x=1}^{19} R_x \right) \tag{10}$$

A random number r is chosen and the particle evaporated in the case at hand selected as the nth, where n is determined by the requirement

$$\sum_{x=1}^{n-1} P_x \leq r < \sum_{x=1}^{n} P_x \tag{11}$$

3.3. According to Weisskopf the normalized spectrum of kinetic energies of an evaporated particle is given by

$$N(\epsilon_x)\, d\epsilon_x = T_x^{-2} (\epsilon_x - k_x V_x) \quad e^{-(\epsilon_x - k_x V_x)/T_x} \; d\epsilon_x , \quad k_x V_x \leq \epsilon_x < \infty . \tag{12}$$

$T_x$ is a constant depending on the level density of the residual nucleus and equal to half the average value of $\epsilon_x - k_x V_x$. The spectrum (12) is only approximate, as mentioned by Dostrovsky; however, it has been used in the present program because it introduces only a slight error compared to the uncertainties already inherent in the theory and because it can be generated easily as follows:

If two random numbers $r_1$ and $r_2$ are distributed according to the exponential distribution, then half their sum, $w = (1/2)(r_1 + r_2)$, is distributed

$4we^{-2w}$ *

according to the distribution ~~$we^{-w}$~~. If $2T_x$ is the average value of $\epsilon_x - k_xV_x$, we then choose

$$\epsilon_x = 2T_x w + k_x V_x \tag{13}$$

for the kinetic energy.

From Eq. 8 it follows that

$$2T_x = [I_2(S) + \beta I_1(S)] \,/\, [I_1(S) + \beta I_o(S)] \quad \text{(neutrons)} \tag{14a}$$

$$2T_x = I_2(S)/I_1(S) \quad \text{(charged particles)} \tag{14b}$$

where

$$I_2(S) = (32a^3)^{-1}\,(8S^3 - 48S^2 + 120S - 120 + e^{-S}\,[S^4 - 12S^2 + 120]) \tag{14c}$$

3.5. After a particle x and its kinetic energy $\epsilon_x$ are chosen, a new compound nucleus is formed according to the equations

$$A' = A - A_x \tag{15a}$$

$$Z' = Z - Z_x \tag{15b}$$

$$U' = U - Q_x - \epsilon_x \tag{15c}$$

4. Operating Instructions

4.1. Immediately following the binary deck is a series of data cards on which Wapstra's nuclear masses are given in the following order:

Col. 1-10: A(I10)

Col. 11-20: Z(I10)

Col. 21-30: Mass excess with sign in Mev (E10.4)*

*The parenthetic quantities refer to the type of conversion.



*Corrected 3/2/65
BfM

ORNL – AEC – OFFICIAL

At the end of this deck there must appear a single card with a zero punched in Col. 10. The order of the cards in this deck is irrelevant, and any or all of these cards may be withdrawn (except the one with the single zero) or replaced so long as the above format is adhered to.

4.2. Directly following the card with the zero in Col. 10 are to be placed the data cards for the various desired cases. For each case two data cards of the following types must appear:

Card 1

| | |
|---|---|
| Col. 1-10: | A(I10) |
| 11-20: | Z(I10) |
| 21-30: | Number of histories (I10) |
| 31-40: | First output option integer, I, which can equal 1,2, or 3 (I10) |
| 41-50: | Second output option integer, J, which can equal 1 or 2 (I10) |
| 51-60: | Case number (I10) |

Card 2

| | |
|---|---|
| Col. 1-10: | U, the excitation energy of the initial compound nucleus in Mev (E10.2) |
| 11-20: | Y (see Eq. 3) (E10.2) |
| 21-30: | B (see Eq. 3) in Mev (E10.2) |

These card pairs are simply placed one behind the other.

4.3. The output format is as follows: At the top of the first page all the input data except for the two output option integers are printed. In the middle of this page the total numbers of each of the different kinds of particles evaporated are printed out. If I = J = 1, this first page alone comprises the entire output. If either I or J $\neq$ 1, more information is printed out. When this happens, the first thing to appear on every succeeding page of output is the case number. In this way output pages corresponding to various cases may be separated and filed as desired with no danger of confusion.

4.4. Each history ends on a final nucleus stable against particle emission. If J = 2 the number of each kind of final nucleus occurring is printed out, all isobars appearing on one page and no two on the same page. Only final nuclei with a mass number within 70 mass units and a charge number within 35 charge units of the initial compound nucleus are recorded. All those lying outside these limits are not recorded; their total number, however, is printed out on the page following the listing of final nuclei.

4.5. If I = 2, the neutron kinetic energy spectrum is printed out following the listing of final nuclei when it is present or directly after the first page otherwise. The spectrum is in the form of a tabular histogram with an interval width of 0.1 Mev. Only kinetic energies $\leq$ 50 Mev are recorded. When I = 3, six spectra with this same format are printed out; the labeling 1 through 6 has the following meaning: 1 = neutron, 2 = proton, 3 = deuteron, 4 = triton, 5 = $He^3$, 6 = alpha particle.

4.6. In addition to any output specified by these options, the details of each history may be printed out by punching any integer in columns 61-70 of data card 1. This will cause the following information to be printed out for each particle emitted:

1) The mass and charge numbers (A,Z)* of the emitting nucleus.

2) The excitation energy (U) in Mev of the emitting nucleus.

3) An integer (JEMISS) from 1 to 19 specifying the kind of particle emitted. These integers correspond to the possible particles as follows (asterisks denote excited states):

| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | |
|---|---|---|---|---|---|---|---|---|---|
| n | $H^1$ | $H^2$ | $H^3$ | $He^3$ | $He^4$ | $He^6$ | $Li^6$ | $Li^{6*}$ | |
| **10** | **11** | **12** | **13** | **14** | **15** | **16** | **17** | **18** | **19** |
| $Li^7$ | $Li^{7*}$ | $Be^7$ | $Be^{7*}$ | $Li^8$ | $Li^{8*}$ | $Li^9$ | $Be^9$ | $Be^{10}$ | $Be^{10*}$ |

4) The average kinetic energy $2T_x$ in Mev (EPSAV)

5) The actual kinetic energy $\epsilon_x$ in Mev (EPS)

6) The random numbers r(URAN), $r_1$(E1),and $r_2$(E2).

7) The binding energies $Q_x$(Q), x = 1,19

8) The quantities $Q_x + k_x V_x$ (THRESH), x = 1,19

9) The quantities $R_x$(R) and the related average emission probabilities $P_x$(P), x = 1,19

10) The constants $k_x$(FLKCØU) and $C_x$(CCØUL), x = 1,19

This information, together with the case number, is printed on a separate page for each emitted particle. If many cases are considered under this output regimen, the print-out may become prohibitively long.

The author gratefully acknowledges the help of Mr. J. G. Sullivan.

---

*The parenthetic expressions denote the names given to the various quantities in the print-out.

## References


1. V. F. Weisskopf, Phys. Rev. 52 295 (1937).

2. K. J. LeCouteur, "Nuclear Reactions," Vol. I, ed. by P. M. Endt and M. Demeur, North Holland Publishing Co., Amsterdam, 1958, Ch. VII.

3. I. Dostrovsky, Z. Fraenkel and G. Friedlander, Phys. Rev. 116 683(1959); I. Dostrovsky, Z. Fraenkel and L. Winsberg, Phys. Rev. 118 781 (1960); I. Dostrovsky, Z. Fraenkel and P. Rabinowitz, Phys. Rev. 118 791 (1960).

4. J. M. Blatt and V. F. Weisskopf, "Theoretical Nuclear Physics," Wiley and Sons, New York, 1952, p. 371.

5. K. J. LeCouteur and D. W. Lang, Nucl. Phys. 13 32 (1959).

6. A. G. W. Cameron, Can. J. of Phys. 36 1040 (1958).

7. A. M. Wapstra, Physica 21 367, 385 (1955).

8. J. R. Huizenga, Physica 21 410 (1955).

9. A. G. W. Cameron, Can. J. of Phys. 35 1021 (1957).