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EVAP-2 AND EVAP-3: MODIFICATIONS OF A
CODE TO CALCULATE PARTICLE EVAPORATION
FROM SELECTED COMPOUND NUCLEI

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EVAP-2 and EVAP-3: Modifications of a Code to Calculate
Particle Evaporation from Excited Compound Nuclei

M. P. Guthrie

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TABLE OF CONTENTS

	Page No.
ABSTRACT	1
I. INTRODUCTION	2
II. EVAP-2	3
Description of Calculation	3
Modifications Incorporated in EVAP-2	4
Updated EVAP Table Tape	4
⁸ Be Breakup	5
Negative Excitation Energies	5
Additional Minor Modifications	6
Input Requirements	6
Subroutine Structure	7
Sample Case	8
III. EVAP-3	14
Differences Between EVAP-2 and EVAP-3	14
Calculation of Kinetic Energies of Recoiling Nuclei in EVAP-3	15
Input Requirements and Subroutine Structure	17
Sample Case	17
ACKNOWLEDGMENTS	24
REFERENCES	25

EVAP-2 and EVAP-3: Modifications of a Code to Calculate
Particle Evaporation from Excited Compound Nuclei

M. P. Guthrie

Abstract

The EVAP computer programs calculate the types, multiplicities, and energy distributions of particles evaporated from excited compound nuclei. The modifications incorporated in EVAP-2 include updating the nuclear masses and shell-plus-pairing energy corrections used as input data, providing for the breakup of ^8Be , and eliminating the possibility of the evaporation residual nucleus having a negative excitation energy. EVAP-3 retains all of the modifications of EVAP-2 and, in addition, calculates the kinetic energies of the recoiling nuclei. The codes are written in FORTRAN-IV and operate on the IBM-360 computer. Data cards and the printed output for a sample case are shown.

I. INTRODUCTION

Dresner's Monte Carlo computer program EVAP¹ determines the types, multiplicities, and energy distributions of particles evaporated from excited compound nuclei. This useful calculation has been modified many times and is often used in association with other calculations including Bertini's intranuclear-cascade codes LECC and MECC² and the nucleon transport code NTC.³ EVAP-2 and EVAP-3 operate without other codes. The evaporation process is started by the collision of an incident particle with a target nucleus. An excited compound nucleus is formed, from which particles are emitted until evaporation is no longer energetically possible. The physics in EVAP-2 and in EVAP-3 is identical to that in the evaporation codes used by the cascade calculations and NTC. The only difference in the two sets of codes is in the formation of the compound nucleus. In EVAP-2 and -3 the compound nucleus is formed directly, while in the other codes it is formed at the end of the intranuclear cascade.

EVAP-2 was written to update the input data used by the evaporation calculation and to incorporate the most desirable modifications of earlier versions into one "standard" code. EVAP-3 was originally written to be used with the low-energy cascade calculation to study the effects of the capture of negative pions in light elements.⁴ It is identical to EVAP-2 in all respects except that the effects of the kinetic energies of the recoiling nuclei are included in the calculation. The two codes operate on the IBM-360 computer and are written in FORTRAN-IV. The subroutines that generate random numbers are in machine language.

II. EVAP-2

DESCRIPTION OF CALCULATION

Dresner's original calculation began with a compound nucleus of predetermined type and excitation energy. EVAP-2 begins one step earlier with the collision of a particle of predetermined type and kinetic energy with a stationary nucleus. The compound nucleus formed by this collision is determined simply by adding the mass and charge of the incident particle to the mass and charge of the target nucleus. The excitation energy of the compound nucleus is the sum of the kinetic energy of the incident particle and the binding energy of the incident particle in the compound nucleus.

After the determination of the type and excitation energy of the compound nucleus, EVAP-2 follows Dresner's evaporation calculation very closely except that only 6 types of evaporated particles are considered instead of Dresner's original 19. The calculation is based on a theory originally proposed by Weisskopf⁵ and on a Monte Carlo code written by Dostrovsky.⁶ The calculation is clearly explained in Dresner's description of his code.¹

Seven types of incident particles can be used in EVAP-2: neutrons, protons, deuterons, tritons, helium-3 nuclei, alpha particles, and photons. The first six types of these particles can be evaporated from the excited compound nucleus. The output data include a table of the distribution of residual nuclei following evaporation and, for each type of evaporated particle, the average evaporation yield per collision, the moments of the energy distributions, and tables of normalized energy spectra.

MODIFICATIONS INCORPORATED IN EVAP-2

Updated EVAP Table Tape

The nuclear masses used by EVAP were obtained from tables compiled by Wapstra⁷ and Huizenga.⁸ Mattauch *et al.*⁹ have recently published a new tabulation of mass excesses and binding energies. The mass excesses in the new tabulation are based on an atomic mass unit of 1/12 of ¹²C. Since the data used in EVAP are based on ¹⁶O, the binding energies tabulated by Mattauch *et al.* were used rather than the mass excesses. The binding energies were converted to mass excesses on the EVAP Table Tape using the formula:

$$\text{EMEX} = Z * (\text{EMH} - \text{EMN}) + A * (\text{EMN} - \text{UM}) - \text{BE}$$

where

EMEX = mass excess in MeV

Z = charge of nucleus

A = mass number of nucleus

EMH = 938.7298, mass of proton in MeV

EMN = 939.5124, mass of neutron in MeV

UM = 931.145, unit mass in MeV

BE = binding energy in MeV tabulated by Mattauch *et al.*

For nuclei not tabulated by Mattauch *et al.* but having a mass number within + 10 of the valley of stability of the periodic table, mass excesses were calculated using the semiempirical mass relationship of Cameron.¹⁰ These were stored along with the Mattauch *et al.* data in the WAPS array on the new EVAP Table Tape in the same manner as they were stored on the previously used tape.

Cameron's mass relationship uses a set of "shell-plus-pairing" energy corrections, which are stored as Cameron Functions on the EVAP Table Tape. Cameron listed no values for these corrections for nuclides with Z or N less than 11. Cameron Functions for small Z or N were therefore set equal to zero on the original EVAP Table Tape. Peelle and Aebersold¹¹ observed that large mass errors could be made using the zero Cameron Functions for light nuclides. They obtained new values for the shell-plus-pairing energy corrections for nuclides with Z or N less than 11 using a weighted least-squares fit to Mattauch *et al.*'s masses. These new values have replaced the zeros in the Cameron Functions on the new EVAP Table Tape.

⁸Be Breakup

When a ⁸Be nucleus is formed in the evaporation process, it will split into two alpha particles instead of evaporating a lighter particle. This fact was ignored in the original EVAP calculation but has been taken into account in EVAP-2. If an evaporation residual nucleus has an A value of eight and a Z value of four, it is assumed that two alpha particles are created. Each alpha particle has an energy equal to one-half the sum of the excitation energy of the ⁸Be nucleus and the binding energy for the reaction. These alpha particles are then treated as evaporation particles with no further evaporation taking place. A counter records the number of times ⁸Be breakup occurs.

Negative Excitation Energies

Because of the Monte Carlo sampling techniques used in the evaporation calculation, it is possible for the kinetic energy selected for the evaporated particle to be greater than the energy available for the reaction. This results in a negative excitation energy for the evaporation residual

nucleus. If this happens in EVAP-2, the calculation recycles and a new kinetic energy is selected for the evaporated particle. If a physically reasonable energy has not been obtained in ten attempts, the evaporation process is terminated at the previously evaporated particle.

Additional Minor Modifications

In the tables of evaporation residual nuclei printed out by EVAP, residual nuclei were sometimes identical to evaporated particles when light target nuclei were studied. These nuclei were not included in the multiplicities of the evaporated particles and their energies were not indicated in the energy spectra. EVAP-2 tests the final evaporation residual nucleus. When it is identical to one of the six types of evaporated particles, it is treated as an evaporated particle and not as a residual nucleus. A count is kept of the residual nuclei with changed status, so that all residual nuclei are accounted for.

INPUT REQUIREMENTS

Only one input data card is required to operate EVAP-2. The card format is 3I15, F15.0, I15. The five input variables are as follows:

- NATA - the mass of the target nucleus;
- NZTA - the charge of the target nucleus;
- ITYPE - the type of incident particle specified by the following code:
 - 1, neutron; 2, proton; 3, deuteron; 4, triton; 5, ^3He nuclei;
 - 6, alpha particle; 7, photon;
- EKIN - the kinetic energy of the incident particle in MeV;
- IHISNO - the number of incident-particle collisions to be calculated.

The remaining input data are stored on a magnetic tape referred to as the EVAP Table Tape. The tape has the logical number 3 in the calculation.

Any number of cases may be run in succession by simply placing additional data cards behind the first one.

The evaporation calculation always begins with the same random number, so that the same cases run at different times should be identical. However, if more than one case is run in succession, all cases after the first begin with the last random number generated in the preceding case.

SUBROUTINE STRUCTURE

EVAP-2 consists of a main program and six subroutines. Two of the subroutines, FLTRN and EXPRN, are machine language programs to generate random numbers. The main program reads the input tape, does only a few minor calculations, calls DRES, and writes the output tape.

DRES is the subroutine in which the major part of the calculation is carried out. There are three calls to DRES from the main program. On the first call, data are read into the memory from the EVAP Table Tape. On the second call, information from the input tape is transferred to DRES, and appropriate variables are zeroed. On the third call, the Monte Carlo evaporation calculation is performed for the first incident particle. The third call is repeated for the number of incident-particle collisions specified on the data card. If more than one case is run in succession, the first call to DRES is not repeated since the data on the EVAP Table Tape are the same for all cases.

THRES is a function subprogram that calculates the binding energy for the formation of a compound nucleus from the collision of the incident particle with the target nucleus. THRES is not called for incident photons. The excitation energy of the compound nucleus is simply the kinetic energy of the photon in this case.

EVAP-2
A OF TARGET = 56
Z OF TARGET = 26
KINETIC ENERGY (MEV) = 18.00
INCIDENT PARTICLE = PROTON
EXCITATION ENERGY = 24.02
CASE HISTORIES = 4000

AVERAGE EVAPORATION YIELD PER INELASTIC EVENT

NEUTRONS	PROTONS	DEUTERONS	TRITONS	HE3	ALPHAS
0.672000	0.655750	0.0	0.0	0.0	0.004250

NUMBER OF HISTORIES IN WHICH BERYLLIUM-8 BREAKUP OCCURRED 0

NUMBER OF HISTORIES IN WHICH A RESIDUAL NUCLEUS WAS IDENTICAL TO ONE OF THE SIX SPECIES OF PARTICLES WHOSE SPECTRA ARE GIVEN BELOW 0

CASE NUMBER 56 26 18 2

DISTRIBUTION OF RESIDUAL NUCLEI FOLLOWING EVAPORATION

A	Z	NUMBER OF NUCLEI	EXCITATION ENERGY (MEV)
56	27	1337	9.1483
	26	518	11.2193
55	27	23	1.6879
	26	2105	1.9425
53	25	17	7.0494

AVERAGE EXCITATION ENERGY OF RESIDUAL NUCLEI 5.5727

III. EVAP-3

DIFFERENCES BETWEEN EVAP-2 AND EVAP-3

The evaporation calculation in EVAP-3 is identical to that in EVAP-2 except that the effects of nuclear recoil are included in EVAP-3. EVAP-2 assumes that the initial excited nucleus is fixed and ignores recoil velocity. The same assumption is made for a nucleus after the evaporation of a particle, allowing all of the energy of the nucleus to be available as excitation energy for the next evaporation. This means, in effect, that EVAP-2 neglects the difference between the laboratory and center-of-mass systems.

In EVAP-3 the excitation energy used to calculate the evaporation of the first particle from the original compound nucleus is the energy available in the center-of-mass system. Before evaporation, the velocity of the center-of-mass system is equated to the recoil velocity of the compound nucleus. After each evaporation, the velocity of the new residual nucleus is calculated, and this becomes the velocity of the center of mass for the next evaporation.

In EVAP-2 the particles are assumed to be evaporated isotropically from the excited nuclei. In EVAP-3 the particles are evaporated isotropically in the center-of-mass system. The distribution in the laboratory system is therefore no longer isotropic.

In general, the differences in the results calculated by the two codes are small. The particle multiplicities are, on the average, slightly lower in EVAP-3 and therefore the residual nuclei are slightly heavier.

CALCULATION OF KINETIC ENERGIES OF RECOILING NUCLEI IN EVAP-3

The first step in determining the recoil kinetic energy of the original compound nucleus is the calculation of the momentum of the incident particle. Since the target nucleus is assumed to be stationary, the momentum of the compound nucleus was equated to that of the incident particle. The kinetic energy of the compound nucleus was then determined from the momentum, and this value was subtracted from the excitation energy of the compound nucleus calculated by the method of EVAP-2.

To calculate the recoil kinetic energy and the excitation energy of each evaporation residual nucleus, the following symbols are used (primed quantities refer to the center-of-momentum system and unprimed quantities refer to the laboratory system):

E^* = the excitation energy of the evaporation residual nucleus;

\overline{v}_c = the velocity of recoil nucleus before evaporation, which is also equal to the velocity of the center-of-momentum system after evaporation;

\overline{v}_i' = the velocity of the next evaporated particle of type i in the center-of-momentum system;

\overline{v}_r' = the recoil velocity of the nucleus after emission of particle i in the center-of-momentum system;

M_r = the mass of nucleus after emission of particle i ;

M_i = the mass of evaporated particle i ;

θ = the angle in the center-of-momentum system between \overline{v}_i' and \overline{v}_c ;
 $\cos\theta$ is selected from an isotropic distribution between 0 and 180° .

The velocities of the evaporated particle and the recoil nucleus in the laboratory system may be expressed as follows:

$$\overline{v}_i = \overline{v}_i' + \overline{v}_c$$

$$v_i^2 = v_i'^2 + v_c^2 + 2v_i' v_c \cos\theta$$

$$\overline{v}_r = \overline{v}_r' + \overline{v}_c$$

$$v_r^2 = v_r'^2 + v_c^2 + 2v_r' v_c \cos(180 + \theta) ,$$

and, in the center-of-momentum system,

$$M_r \overline{v}_r' = M_i \overline{v}_i' ;$$

therefore,

$$v_r'^2 = (M_i/M_r)^2 v_i'^2 .$$

The square of the recoil velocity of the nucleus in the laboratory system is then

$$v_r^2 = (M_i/M_r)^2 v_i'^2 + v_c^2 + 2(M_i/M_r) v_i' v_c \cos(180 + \theta) .$$

The type of evaporated particle and the energy of the evaporated particle are determined using Monte Carlo sampling techniques, and therefore M_i and v_i' can be calculated. v_c can be calculated from the recoil kinetic energy of the original compound nucleus for the first evaporated particle. For subsequent evaporations, v_c is simply the v_r calculated for the previous evaporation.

The excitation energy, E_{new}^* , of the residual nucleus after a particle is evaporated is equal to the excitation energy of the nucleus before evaporation minus the sum of the kinetic energies of the evaporated particle

and the residual nucleus and also minus the binding energy Q of the evaporated particle in the nucleus before evaporation.

$$\begin{aligned} E_{\text{new}}^* &= E^* - \frac{1}{2} M_r v_r'^2 - \frac{1}{2} M_i v_i'^2 - Q \\ &= E^* - \frac{1}{2} [M_r (M_i/M_r)^2 + M_i] v_i'^2 - Q . \end{aligned}$$

The velocity of the evaporated particles in the laboratory system is used to calculate the energies for the energy distributions and spectra tabulated by EVAP-3.

INPUT REQUIREMENTS AND SUBROUTINE STRUCTURE

The input data card and the subroutine structure in EVAP-3 are identical to that in EVAP-2. The printed output is also the same in the two codes except that in the table, "Distribution of Residual Nuclei Following Evaporation," there is one additional column for the tabulation of the recoil kinetic energies of the nuclei.

SAMPLE CASE

The printed output for the same sample case that was used for EVAP-2 is shown for EVAP-3. The data card is identical to the one shown for EVAP-2.

A comparison of the normalized neutron energy spectra calculated by EVAP-2 and EVAP-3 is shown in Fig. 1. Standard deviations are not calculated by the EVAP codes, but the difference between these two spectra is almost surely due to the statistical nature of the calculation.

CASE NUMBER 56 26 18 2

EVAP-3
A OF TARGET = 56
Z OF TARGET = 26
KINETIC ENERGY (MEV) = 18.00
INCIDENT PARTICLE = PROTON
EXCITATION ENERGY = 23.70
CASE HISTORIES = 4000

AVERAGE EVAPORATION YIELD PER INELASTIC EVENT

NEUTRONS	PROTONS	DEUTERONS	TRITONS	HE3	ALPHAS
0.5444995	0.5520600	0.0	0.0	0.0	0.0037500

NUMBER OF HISTORIES IN WHICH BERYLLIUM-8 BREAKUP OCCURRED 0

NUMBER OF HISTORIES IN WHICH A RESIDUAL NUCLEUS WAS IDENTICAL TO ONE OF THE SIX SPECIES OF PARTICLES WHOSE SPECTRA ARE GIVEN BELOW 0

DISTRIBUTION OF RESIDUAL NUCLEI FOLLOWING EVAPORATION

A	Z	NUMBER OF NUCLEI	EXCITATION ENERGY (MEV)	KINETIC ENERGY (MEV)
56	27	1729	9.1702	0.3729
	26	615	11.1121	0.4315
55	27	8	1.7089	0.3328
	26	1633	1.7950	0.3911
53	25	15	5.6501	1.0520

AVERAGE EXCITATION ENERGY OF RESIDUAL NUCLEI 6.4288

MOMENTS OF THE ENERGY DISTRIBUTIONS FOR THE FOLLOWING EVAPORATION PARTICLES

	NEUTRONS	PROTONS	DEUTERONS	TRITONS	HE3	ALPHAS
1ST MOM.	1.94347E 00	4.57761E 00	0.0	0.0	0.0	1.02445E 01
2ND MOM.	6.24790E 00	2.30356E 01	0.0	0.0	0.0	1.06772E 02
3RD MOM.	2.66856E 01	1.31108E 02	0.0	0.0	0.0	1.13145E 03

NORMALIZED EVAPORATION NEUT SPECTRUM
(E SPECIFIES THE LOWER ENERGY LIMIT OF THE INTERVAL IN MEV)

E	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	
0	0.423328	0.408526	0.393724	0.301954	0.316335	0.319716	0.278271	0.307675	0.281232	0.260509																
1	0.222025	0.358700	0.254565	0.254589	0.254529	0.254565	0.301954	0.301954	0.266430	0.313795																
2	0.242747	0.213144	0.224985	0.166501	0.153541	0.180501	0.180580	0.171699	0.156898	0.165779																
3	0.145056	0.124334	0.130255	0.115453	0.100651	0.103612	0.091770	0.091770	0.091770	0.091770																
4	0.065127	0.059207	0.055207	0.076929	0.038464	0.059207	0.029603	0.068088	0.053266	0.026643																
5	0.038484	0.029603	0.026643	0.050484	0.020722	0.020722	0.017762	0.041445	0.014802	0.011841																
6	0.020722	0.023683	0.005921	0.011841	0.011841	0.011841	0.011841	0.014802	0.008881	0.011841																
7	0.008881	0.0	0.014802	0.005921	0.011841	0.0	0.008881	0.005921	0.002960	0.002960																
8	0.002960	0.002960	0.002560	0.002960	0.0	0.0	0.002960	0.0	0.0	0.0																
9	0.002960	0.0	0.005921	0.0	0.0	0.0	0.002960	0.0	0.0	0.0																
10	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0																
11	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0																
12	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0																
13	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0																
14	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0																
15	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0																
16	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0																
17	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0																
18	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0																
19	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0																
20	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0																
21	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0																
22	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0																
23	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0																
24	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0																

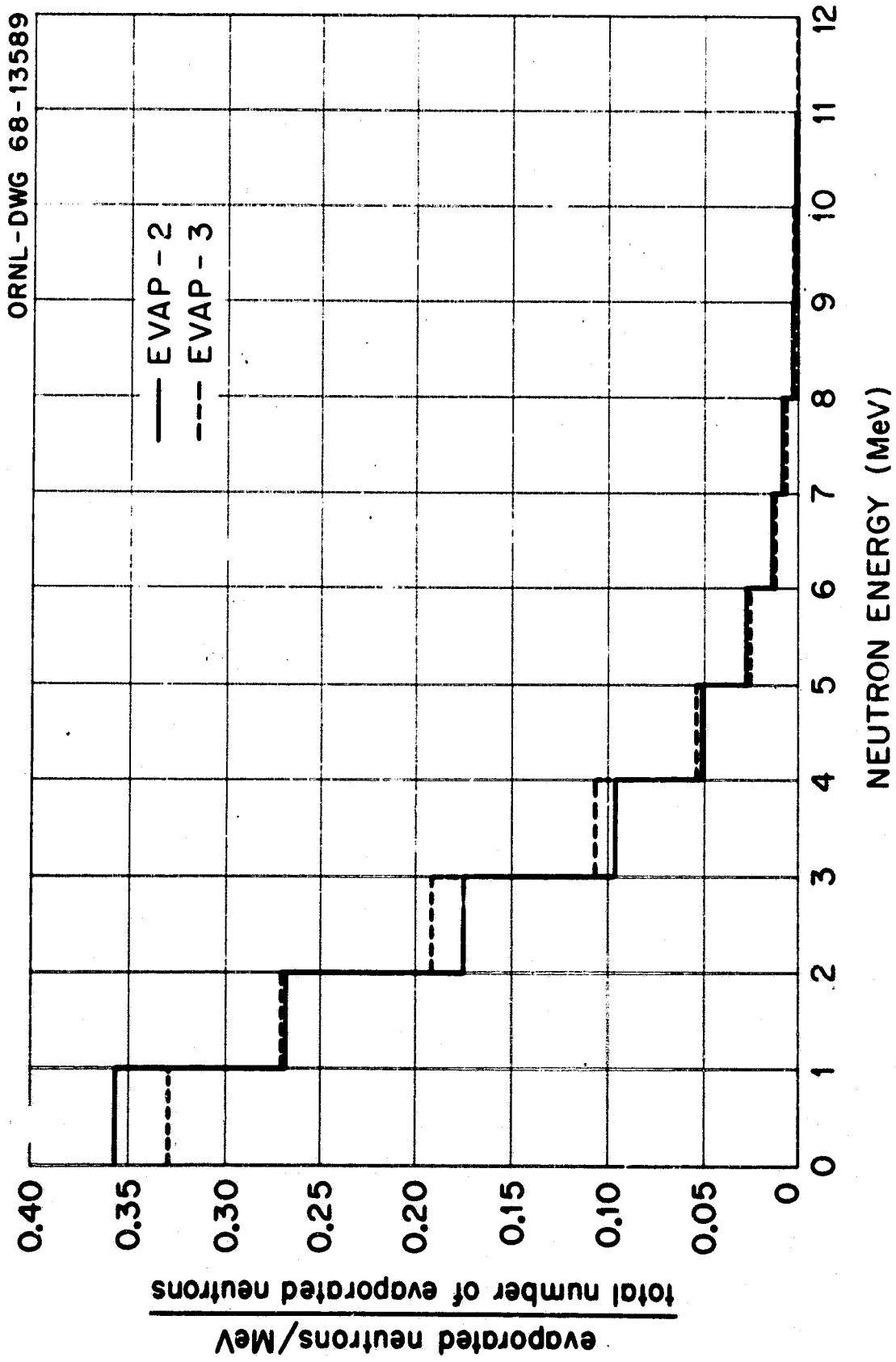


Fig. 1. Normalized Energy Spectra for Evaporation Neutrons.

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