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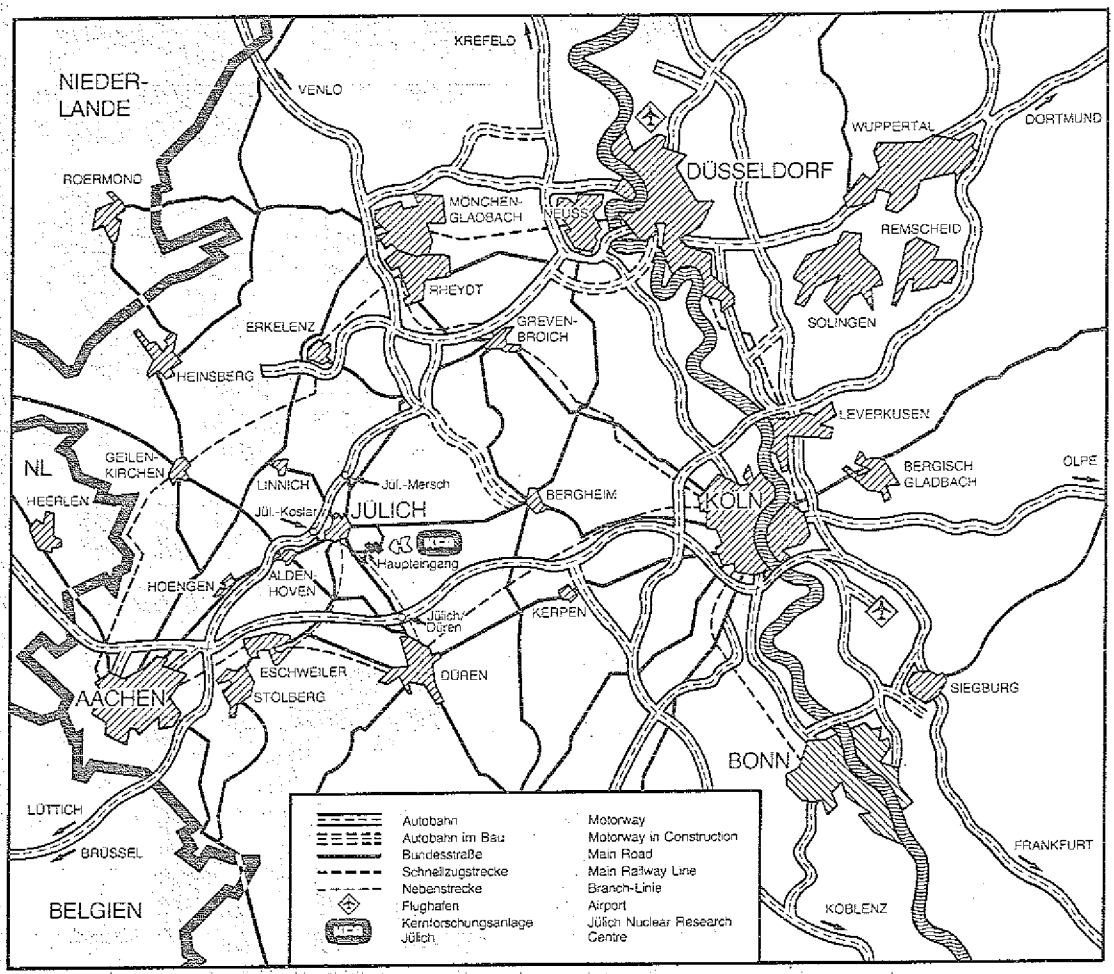

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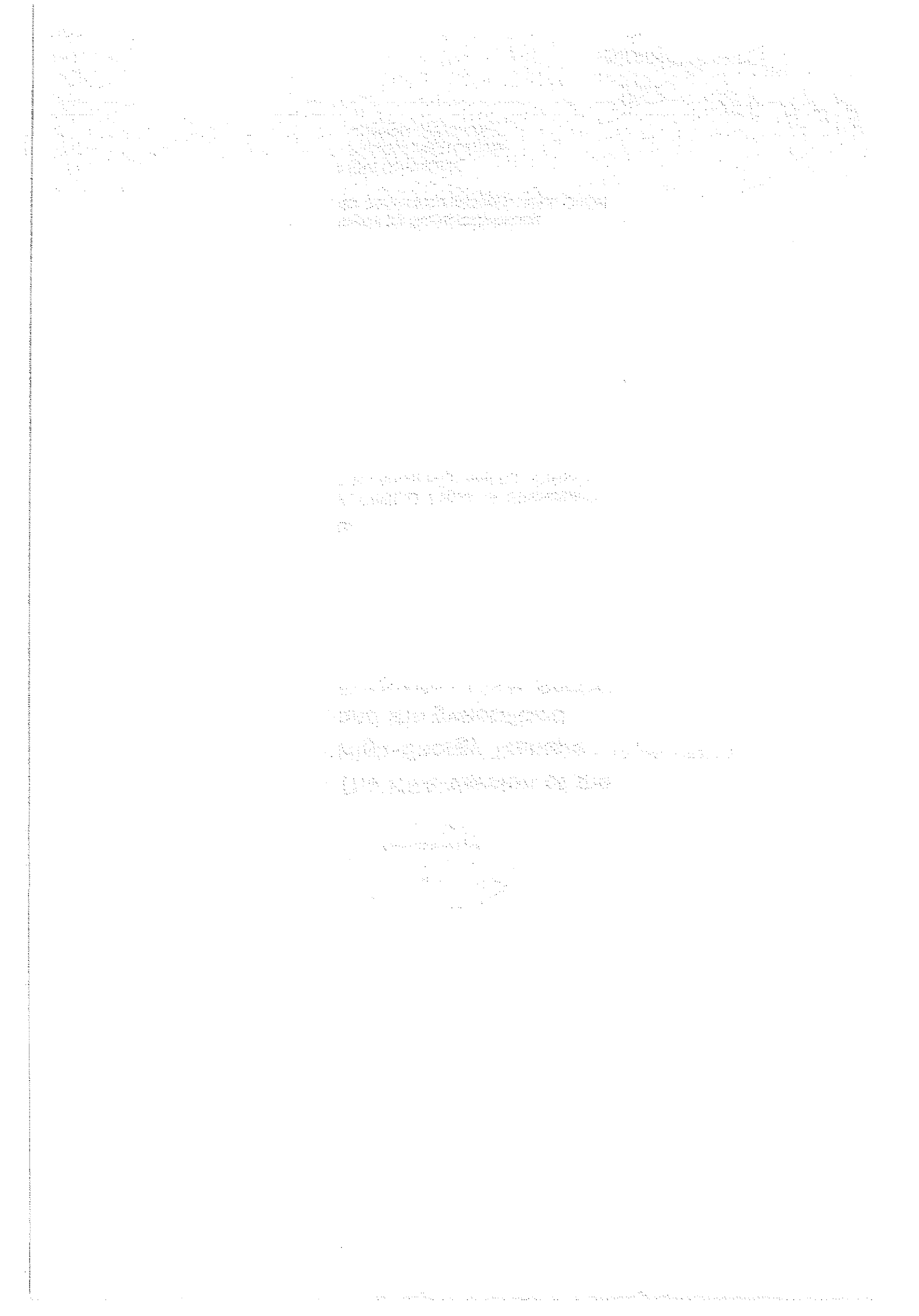

PREFACE

This document describes the updates that have been made to the high-energy transport code HETC for use in the German spallation-neutron source project SNQ. Performance and purpose of the subsidiary code SIMPEL that has been written for general analysis of the HETC output are also described. In addition means of coupling to low energy transport programs, such as the Monte-Carlo code MORSE is provided. As complete input descriptions for HETC and SIMPEL are given together with a sample problem, this document can serve as a user's manual for these two codes.

The document is also an answer to the demand that has been issued by a greater community of HETC users on the ICANS-IV meeting, Oct 20-24 1980, Tsukuba-gun, Japan for a complete description of at least one single version of HETC among the many different versions that exist.

CONTENTS

1 INTRODUCTION

For spallation neutron source applications we are interested in theoretical methods that are capable of predicting a variety of different quantities related to radiation fields produced by proton beams and their associated effects, both in the vicinity of the target station and from beam losses which occur in the accelerator. It is also desirable that such calculational models be sufficiently general to allow investigations of potential applications of spallation sources for purposes in addition to providing an intense low-energy neutron source (e.g., utilization as irradiation facility for radiation effects research, high-energy nuclear physics studies, research related to transmutation and power generation, etc.). To satisfy these needs requires rather general calculational methods which can incorporate numerous physics modules for treating the various types of interaction mechanisms that take place, and which are capable of accommodating complex geometries and material configurations. This necessarily leads to large Monte Carlo computer codes, which is the type of calculational method considered here.

This report is primarily concerned with the programming and documentation aspects of the KFA-IRE system of Monte Carlo codes which have been prepared for use on the KFA IBM-3033 computer. The most essential ones are HETC, MORSE-CG and a newly developed general analysis code SIMPEL for event chains and particle data recorded by HETC. It is assumed here that the reader is familiar with HETC and MORSE-CG. Those readers who are not should read Refs. /1,2,3,4/ and /5/ in conjunction with the present report. Several modifications have been made to the high-energy radiation transport code HETC together with a detailed description of input data used by the intra-nuclear cascade (INC) and evaporation model (not presently available) to arrive at a new version of the code which we have designated HETC/KFA-1. Modifications to HETC are given in chapter 2, a modified input description in chapter 3. The documentation of input data to the intra-nuclear cascade and evaporation code is given in APPENDIX A and APPENDIX B. The analysis code SIMPEL together with its input description is outlined in chapter 4. The MORSE-CG modifications are described in chapter 5. A sample problem is described in APPENDIX E. The modified codes together with the SIMPEL code are available from Institut für Reaktorentwicklung, Kernforschungsanlage Jülich GmbH.

2 MODIFICATIONS TO HETC

2.1 Evaporation Model Modifications

The standard version of the HETC code (i.e., the version distributed by RSIC) contains version 4 of the EVAP evaporation model. The updated version produced here will be refered to as EVAP-5.

2.1.1 Updated Input Data

In the evaporation model calculations, atomic masses are used in determining binding energies. These mass data (in terms of mass excesses) are stored on tape, read as input at the start of each transport calculation, and stored internally as the WAPS array, as defined in APPENDIX A.

EVAP-4 uses the evaluated 1964 Atomic Mass Table values /6/. At present the latest evaluated data are the 1977 Atomic Mass Evaluation by Wapstra and Bos /7/, and it is these data that have been put on the input data tape for EVAP-5.

In the standard EVAP-4, the WAPS (I,J) array was dimensioned WAPS (250,20), with I equal to the mass number of the nuclide J an index defining a particular isotope for a given A, and the following algorithm for retrieval:

$$J = A-2Z-J' + 10$$

$$J' = (A-1)/(1+124/A^{2/3})$$

It was found that this method did not properly represent the new data. That is, the Z and A range for the above method did not cover the range of the input values. In EVAP-5, the WAPS array is dimensioned WAPS (250,11) and WAPS (I,J") denote nuclides with I=A (as before) but J"=1 represents a "starting" Z value for this A. Then WAPS (I,1) corresponds to Z_{min}, WAPS(I,2) corresponds to $Z_{min}+1$, etc. These ten Z values for each A then allow all of the Mass Table values to be contained in the WAPS array, as illustrated in Figs. 1-3.

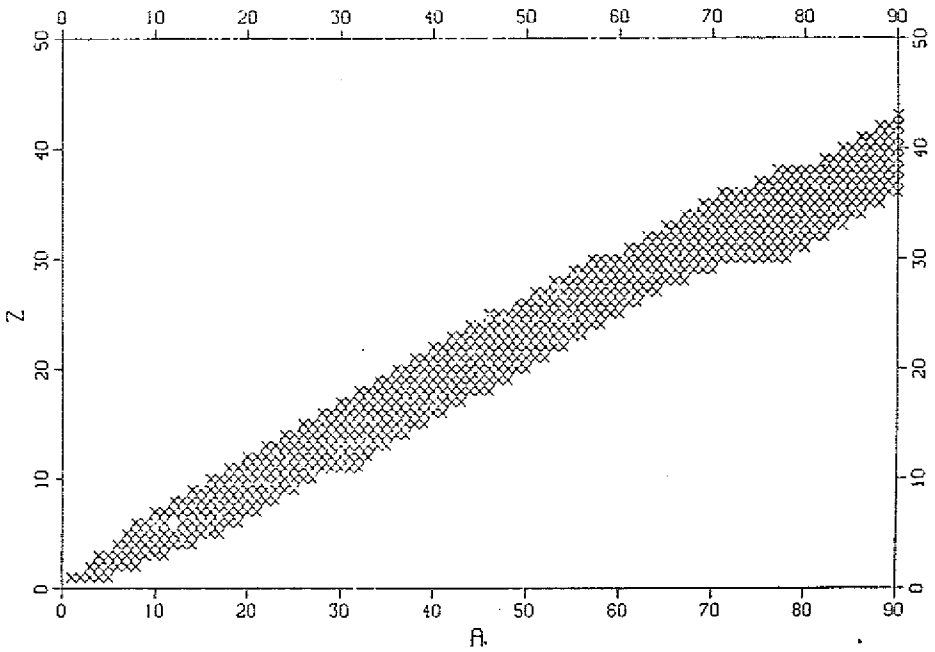

Fig. 1

Nuclide A and Z range covered by updated input data for evaporation model. The symbols denote nuclides for which data are available and stored on the input tape. (Data for A = 1 - 90 shown above; data for higher A in Figures 2 and 3).

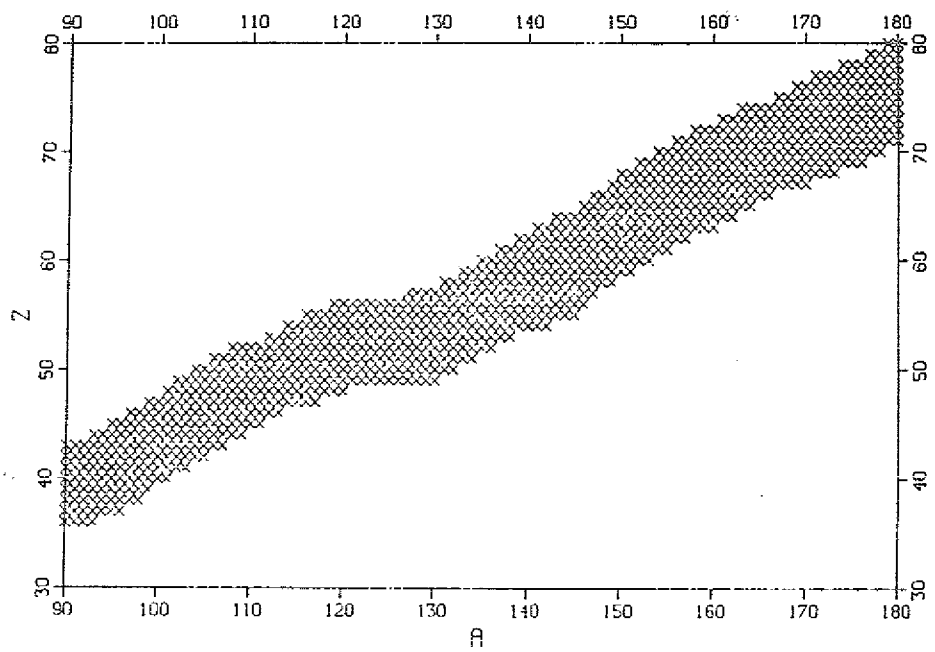

Fig. 2

Nuclide A and Z range covered by updated input data for evaporation model. The symbols denote nuclides for which data are available and stored on the input tape. (Data for A = 90 - 180 shown above; data for higher A in Figure 3).

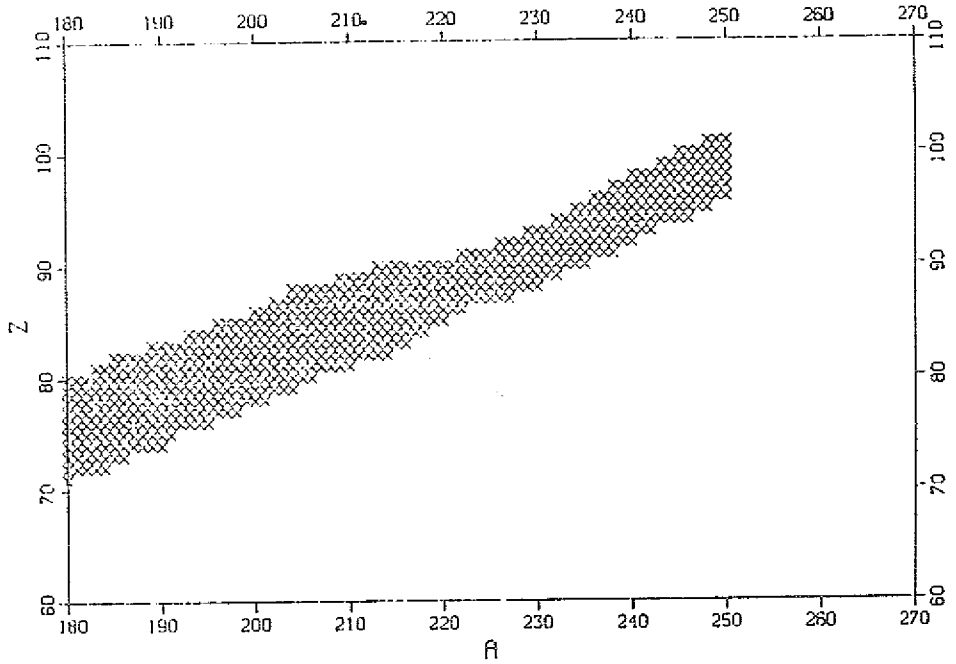

Fig. 3

Nuclide A and Z range covered by updated input data for evaporation model. The symbols denote nuclides for which data are available and stored on the input tape. (Data for A = 180 - 250 shown above).

Another change was made in the procedure used when a nuclide mass is required that is outside of the range of the input data. The binding energy calculation involves the mass difference for two nuclides. In EVAP-4 if input data were not available for one or both nuclides, the Cameron semi-empirical mass formula (discussed in APPENDIX A.) was used. Thus, in computing the mass difference, one mass could be computed from the mass formula and an input value used for the other nuclide. This can lead to what appear to be unrealistic mass differences. Thus, in EVAP-5, a consistent procedure is used -- i.e., if one nuclide is outside of the range of the input data, both nuclide masses are computed using the mass formula. A new function routine,

```
FUNCTION QNRG (A1,Z1,A2,Z2)
```

computes the mass differences using this method.

2.1.2 Level-Density Options Added

In EVAP-4 the level density parameter is computed as

$$a = A/B_0 \ (1+Y\Delta^2/A^2)$$

with B_0=8, Y=1.5, and Δ=A-2Z. The quantity in brackets differs little from unity, so the method assumes a linear mass dependence,

$$a \approx A/B_0 \ MeV^{-1}.$$

From experiments on nuclear level spacing, it is observed that the level density is strongly influenced by nuclear shell structure, with the densities for magic or nearly magic nuclei several orders of magnitude lower than for mid-shell nuclei /8/. Since we are interested in lead targets, an input option has been added to EVAP-5 to use a method for specifying the level density parameter which takes into account shell effects.

Baba /8/ has compiled level densities from neutron resonance measurements for some 200 isotopes. These data are shown in Fig. 4. These values (Table 1) have been stored on the evaporation input data tape as the array APRIME (250), which is read immediately after the WAPS array. An input option allows the above method to be used, or a constant value for B_0 can be input.

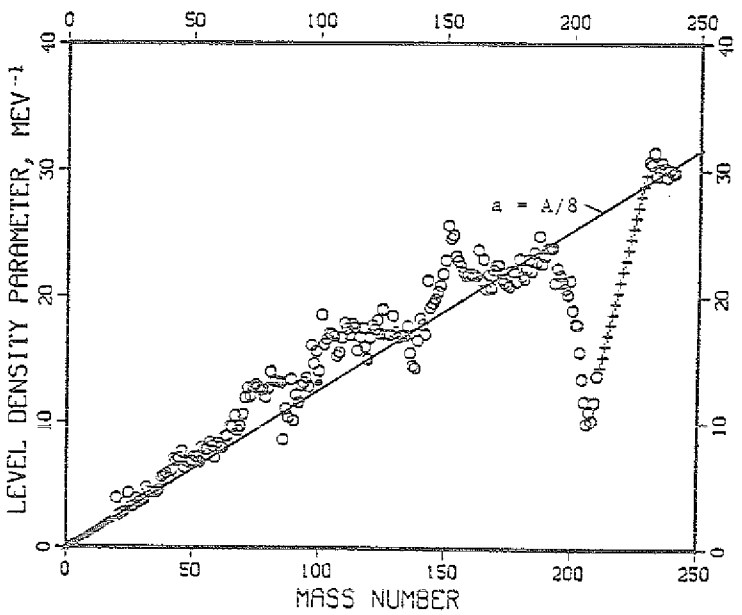

Fig. 4

Level density parameters deduced by Baba /8/ from neutron resonance experiments (circle symbols). The + symbol denotes our rather arbitrary interpolated values for masses not measured. The linear dependence of A/8 is usually assumed in HETC.

Table 1

Level density parameter values used as input for the evaporation model "variable B_Q" option. The integer values are mass numbers and the other numbers are in the corresponding level density parameter values (in MeV^{-1}), as plotted in Fig. 4

1	0.13	2	0.25	3	0.38	4	0.50	5	0.63
6	0.75	7	0.88	8	1.00	9	1.13	10	1.25
11	1.38	12	1.50	13	1.63	14	1.75	15	1.88
16	2.00	17	2.13	18	2.25	19	2.38	20	3.94
21	2.63	22	2.75	23	2.88	24	3.55	25	4.35
26	3.25	27	3.38	28	3.96	29	3.63	30	3.75
31	3.88	32	4.82	33	4.44	34	4.43	35	4.43
36	4.42	37	4.63	38	5.66	39	5.81	40	5.95
41	5.49	42	6.18	43	7.11	44	6.96	45	7.20
46	7.73	47	6.41	48	6.85	49	6.77	50	6.91
51	7.26	52	7.20	53	6.86	54	8.06	55	7.81
56	7.82	57	8.41	58	8.13	59	7.19	60	8.35
61	8.13	62	8.02	63	8.93	64	8.90	65	9.69
66	9.65	67	10.55	68	9.38	69	9.72	70	10.66
71	11.98	72	12.76	73	12.10	74	12.86	75	13.03
76	12.81	77	12.54	78	12.65	79	12.00	80	12.69
81	14.05	82	13.33	83	13.28	84	13.23	85	13.17
86	8.66	87	11.09	88	10.40	89	13.47	90	10.17
91	12.22	92	11.62	93	12.95	94	13.15	95	13.57
96	12.87	97	16.16	98	14.71	99	15.69	100	14.09
101	18.56	102	16.22	103	16.67	104	17.13	105	17.00
106	16.86	107	15.33	108	15.61	109	16.77	110	17.93
111	17.45	112	16.97	113	17.88	114	17.58	115	15.78
116	16.83	117	17.49	118	16.03	119	15.98	120	16.74
121	17.74	122	17.43	123	18.14	124	17.06	125	19.01
126	17.02	127	17.02	128	17.02	129	16.51	130	17.20
131	16.73	132	16.97	133	16.94	134	16.91	135	17.69
136	15.55	137	14.56	138	14.35	139	16.55	140	18.29
141	17.80	142	17.05	143	21.31	144	19.15	145	19.51
146	19.87	147	20.39	148	20.90	149	21.85	150	22.89
151	25.68	152	24.64	153	24.91	154	23.24	155	22.85
156	22.46	157	21.98	158	21.64	159	21.75	160	21.85
161	21.77	162	21.69	163	23.74	164	21.35	165	23.03
166	20.66	167	21.81	168	20.77	169	22.18	170	22.58
171	22.55	172	21.45	173	21.16	174	21.92	175	20.87
176	22.09	177	22.00	178	21.28	179	23.95	180	21.70
181	21.45	182	22.28	183	23.00	184	22.11	185	23.56
186	22.83	187	24.88	188	22.64	189	23.27	190	23.89
191	23.92	192	23.94	193	21.16	194	22.30	195	21.75
196	21.19	197	20.72	198	20.24	199	21.34	200	19.00
201	17.93	202	17.85	203	15.70	204	13.54	205	11.78
206	10.02	207	10.98	208	10.28	209	11.72	210	13.81
211	14.46	212	15.30	213	16.15	214	16.99	215	17.84
216	18.68	217	19.53	218	20.37	219	21.22	220	22.06
221	22.91	222	23.75	223	24.60	224	25.44	225	26.29
226	27.13	227	27.98	228	28.82	229	29.67	230	30.71
231	30.53	232	31.45	233	29.63	234	30.15	235	30.65
236	30.27	237	29.52	238	30.08	239	29.80	240	29.87

2.1.3 Option for Treatment of Emitted-Particle Angular Distributions

In the standard HETC code using the EVAP-4 model, emitted evaporation particles are assumed to be isotropic in the laboratory system. There are two effects which can cause the actual distribution to be non-isotropic: (a) for high bombardment

energies, the nucleus which evaporates the particles can have rather large angular momentum, and (b) the evaporating nucleus is in movement during particle emission with a certain recoil energy. The dominate effect on emitted angular distribution is the nuclear recoil rather than angular momentum /9/. To indicate the general functional dependence and magnitude of anisotropy, an approximate relationship for the angular distribution (in lab system) of evaporated neutrons is /9/

$$W(\theta) \approx 1 + (v^*/v)\cos\theta$$

where v is the neutron velocity and v* is the center-of-mass velocity. As an example, for 600 MeV protons incident on a lead nucleus, the angular distribution of 1-MeV neutrons then is $W(\theta)=1+0.23\cos\theta$, so the $W(0^o)/W(90^o)$ anisotropy is roughly 20% for this case, and larger for lighter nuclei.

Los Alamos has recently modified their version of HETC to take into account the recoil direction of the residual nucleus during evaporation. Evaporated particle directions are selected from an isotropic center-of-mass distribution, and this angle and the recoil direction are transformed to give non-isotropic angular distributions in the laboratory system. These modifications were kindly provided to us by R.E. Prael of Los Alamos, and have been incorporated in the HETC/KFA-1 code as an option. This required changes to the following subroutines: MAIN, DATAHI, ERUP, RECOIL, DRES, and WTAPE. If this option is selected, the direction cosines U, V, and W are written on the history tape for each evaporated particle. We have made only a few runs using this option; it seems to work properly but has not been throughly tested. It should be noted that this option is available at present only when using EVAP-5; it is not incorporated in the RAL fission model.

2.1.4 Option for high-Energy Fission

The way, high energy fission is incorporated in HETC/KFA-1 is outlined in Fig. 5. The high-energy fission model of the Rutherford and Appleton Laboratories developed by F. Atchison was implemented in the code /10/. To complete the documentation of the system a short overview is given. From the intranuclear cascade we get the high energy products plus the residual nucleus which is in a highly exited state. Next the question is whether or not it is undergoing high energy fission. If not, a particle is evaporated (i.e. a neutron, proton etc.) and the

same question is asked again for the remaining, still excited nucleus. In this way all steps of de-exitation are treated. On occurence of fission, two excited nuclei are produced which then decay again by evaporation. In other words, the fission neutrons come from exactly the same processes as the other evaporation neutrons, except that the masses of the evaporating nuclei are lower (see Fig. 5). The problem in implementing a code in HETC which takes fission into account is, of course, that one has to make some decisions, namely whether or not fission is to occur and what will be the scission parameters of the fragments (mass, charge, recoil, excitation).

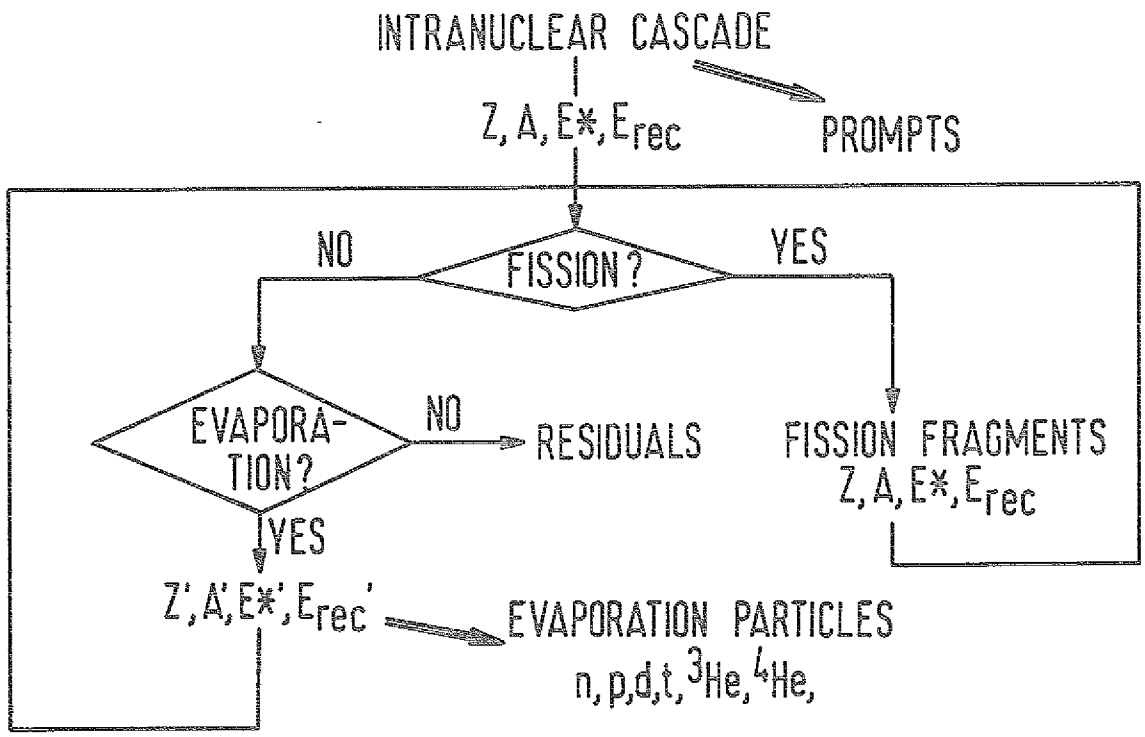

Fig. 5

Sequence of events in a particle-nucleus interaction as modified to include fission /10/.

The choice of parameters are done in the following way:

Fission Probability:

a) Actinide Region Z>88

Fission probabilities rise very rapidly to a fairly constant (<1.0) value. This "saturation" value is reached at 6 MeV excitation in most cases /11/. Fission probabilities in the saturation region are taken from the systematics of Vandenbosch and Huizenga /12/:

$$\log \frac{\Gamma_n}{\Gamma_f} = \Phi(z)A + \psi(z)$$

Γ_n and Γ_f are the widths for neutron emission and fission, A is the mass number of the fissioning system. In the RAL model it is assumed $P_f=0$ for $E^* \leq 6$ MeV and $P_f=(1+\Gamma_n/\Gamma_f)^{-1}$ for $E^*>6$MeV. The Γ_n/Γ_f values are calculated using the tabulated values of $\Phi(z)$ and $\psi(z)$.

b) Subactinide Region Z<88

A statistical fit was made to experimental data and an estimation of the fission probability for given Z, A, E* and the mass-difference table. The fit was made in a way allowing for separate level-density parameters for neutron emission and fission, and a fission barrier which fits the available data. Both the saddle-point level-density parameters and the fission barrier show a systematic variation with the fissionability parameter Z^2/A. The expressions for subactinide fission in the RAL model are (for nucleus Z, A excited to E*):

$$\Gamma_n=0.3518099\ (1.66I_0+1.93\ A^{1/3}\ I_1+A^{2/3}(0.76I_1-0.05I_0))$$

with $$I_0=(2a_n)^{-1}\{(S_n-1.0)e^{S_n}+1.0\}$$

$$I_1=(8a_n^2)^{-1}\{(60-6.0S_n+2.0S_n^2)e^{S_n}+S_n^2-6.0\}$$

$$S_n=2.0\sqrt{a_n(E^*-BE')}$$

Originally used in the RAL Model for the level-density:

$$a_n=(A-1.0)/8.0$$

with fixed $B_0=8$ MeV

(BE'=Separation energy - pairing energy computed by HETC function ENERGY)

$$\Gamma_f=((S_f-1.0)e^{S_f}+1.0/)a_f$$

$$S_f=2.0\sqrt{a_f(E^*-E_f')}$$

$$E'_f=BE'+321.175-16.70314Z^2/A+0.2185024(z^2/A)^2$$

$$a_f/a_n=1.089257+0.01097897(z^2/A-31.08551)^2$$

hence $$P_f=1.0/(1+\Gamma_n/\Gamma_f)$$

Post-Fission Parameters

a) Mass

Let Z,A and E'^* be the actual charge, mass and exitation energy of the actual fissioning nucleus, respectively. For $Z^2/A \leq 35$ the masses A_1 and A_2 of the fission fragments are sampled symmetrically (systematics by Neuzil and Fairhall /13/) from a Gaussian distribution with mean value A/2 and width

$$\sigma_A=-2.12\ 10^{-3}U^2+0.425U+3.97$$

where $U=E'^*-E'_f$ is the exitation above the fission barrier E_f for $Z \leq 88$ (see above) or with $E'_f=C^*-0.36Z^2/A$ for $Z>88$. ($C^*=18.8,18.1,18.1,18.5$ for odd-odd, even-odd, odd-even and even-even nuclei). For $Z<88$ E_f is calculated using the expression given earlier under the fission probability calculation. If $Z^2/A>35$ competition between symmetric ans asymmetric fission is allowed, with the asymmetric probability being

$$P_{as}=F/(1+F),\ F=4870\exp(-0.36E'^*).$$

For asymmetric fission, A_1 is selected from a Gaussian of of mean $\overline{A}=140$ and width $\sigma_A=6.5$, and $A_2=A-A_1$.

b) Charge

The charge of the first fragment Z_1 is selected from a Gaussian distribution of mean $\overline{Z_1}$ and width

$$\sigma_Z=2,\ \text{where } Z_1=(Z+Z'_1-Z'_2)/2$$

$$Z'_i=65.5A_i/(2\cdot 65.5+A_i^{2/3}),\ \text{then } Z_2=Z-Z_1.$$

As an example for the fission probability computed using the RAL model for various isotopes Fig. 6 is attached.

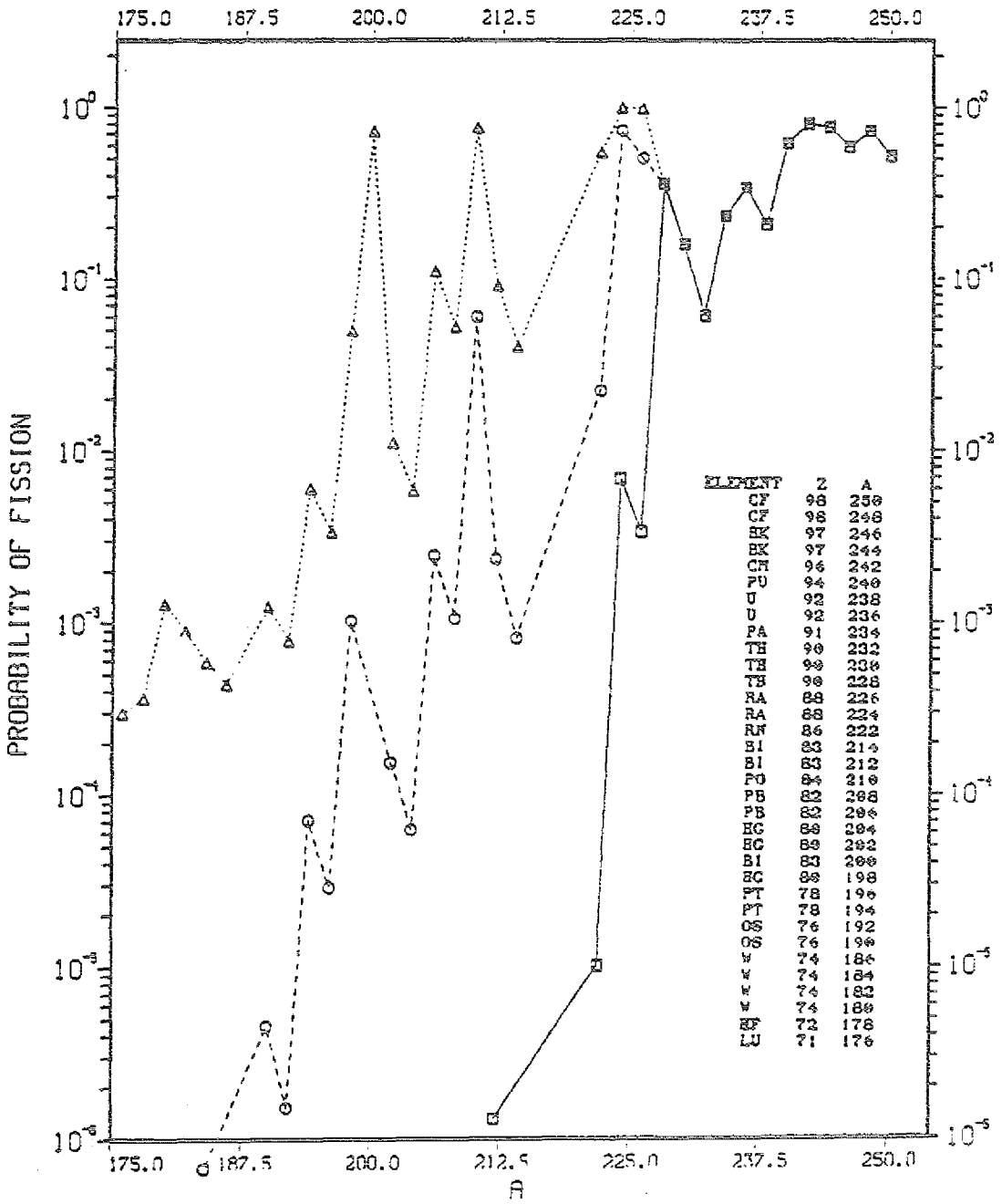

Fig. 6

Probability of fission using RAL model for various isotopes arbitrarily selected over the range from A = 175 - 250. The top, middle, and bottom curves are for assumed excitation energies of 100, 50, and 20 MeV, respectively. (The model assumes that the fission probability is constant for excitation energies above 6 MeV for isotopes having Z above 90).

c) Recoil Kinetic Energy

The total recoil kinetic energy of the fission fragments in the center-of-mass system E_T^* correlates well with the Coulomb repulsion parameter $Z^2/A^{1/3}$. In the model the correlation of Hyde /14/ is used, selected from a Gaussian distribution.

$$E_T^* = 0.13Z^2/A^{1/3} - 11.4$$

and width $\sigma_E = 0.084E_T^*$

d) Excitation

The fragment excitation is computed assuming a uniform distribution of both excitation and binding energy in the fissioning nucleus plus conservation of energy.

2.2 Thick-Target Transport of low-Mass Heavy-Ion Beams

The standard version of the HETC code allows protons, neutrons, π^+, π^-, μ^+, or μ^- as source particles. Previously, modifications were made (for operation on CDC computers) to treat "light" heavy ion beams having $2<A<10$ /15/. The programming for this capability has been converted for operation on IBM computers and incorporated in the HETC-KFA-1 code.

The basic theory is described in Ref. /15/, and only a short summary is given below. The key assumption is that projectile particles can be treated as a cluster of nucleons, and nonelastic interactions computed as the sum of the effects of individual nucleons entering the target nucleus. Interactions then can be computed using the same intranuclear-cascade evaporation model as used for nucleons and pions. This assumption becomes worse as the A of the projectile increases, because for heavier projectiles a cascade can be induced in the projectile particle as well as in the target nucleus. Thus, the model is expected to be applicable for d, t, He, and alpha beams. The A at which the model becomes invalid is not well defined. The programming for the model allows beams up to A=10.

The basic procedure used when a nonelastic collision occurs is as follows:

a) The energy of each nucleon of the projectile is set to $E_N=(E_i-B_i)/A_i$, where E and B are the kinetic and binding energies of the ion. (These binding energies are set internally for A<4, and must be specified as input for A>4)

b) A configuration for the nucleons of the ion is specified. (Fig. 7 shows the configuration assumed for α particles).

c) Impact parameters and a cascade-evaporation calculation is performed sequentially for each nucleon of the cluster.

d) Collisions with hydrogen target nuclei are computed using the same p-p and p-n cross-sections as used by the intra-nuclear cascade code.

e) All atomic processes (ionization energy loss, ranges, etc.) are scaled from relations for protons.

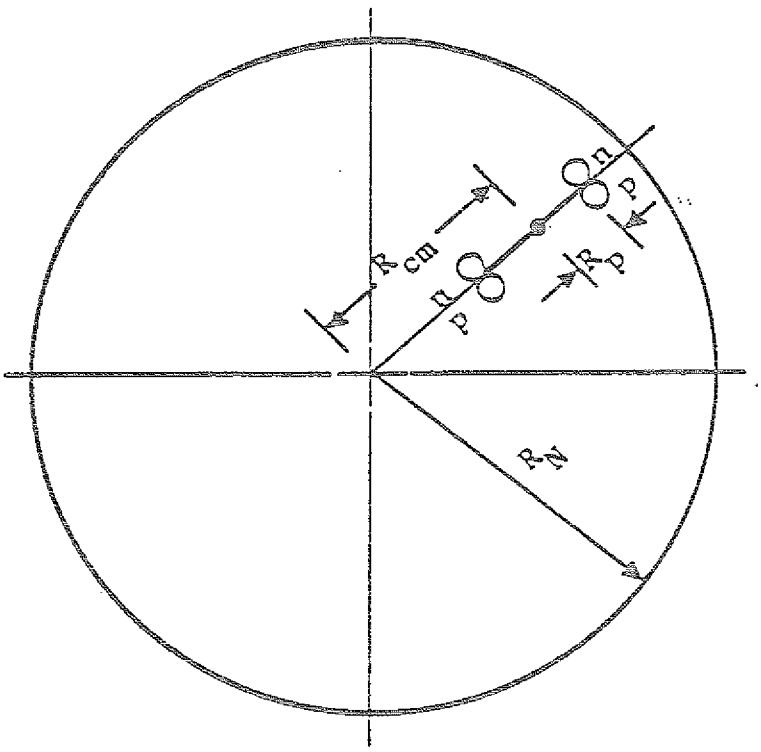

Fig. 7

Determination of impact parameters for individual nucleons of projectile particle incident on target nucleus for heavy-ion interaction model.

R_p = radius of projectile particle
R_N = radius of target nucleus
R_{cm} = radius of projectile center-of-mass incident on nucleus (randomly selected), $0 < R_{cm} < R_N + R_p$

Semi-empirical formulas are used for total ion-nucleus cross-sections. There are no pseudo collisions as in the case of nucleon and pion transport. The additional subroutines for heavy particle transport are indicated in Fig. 8.

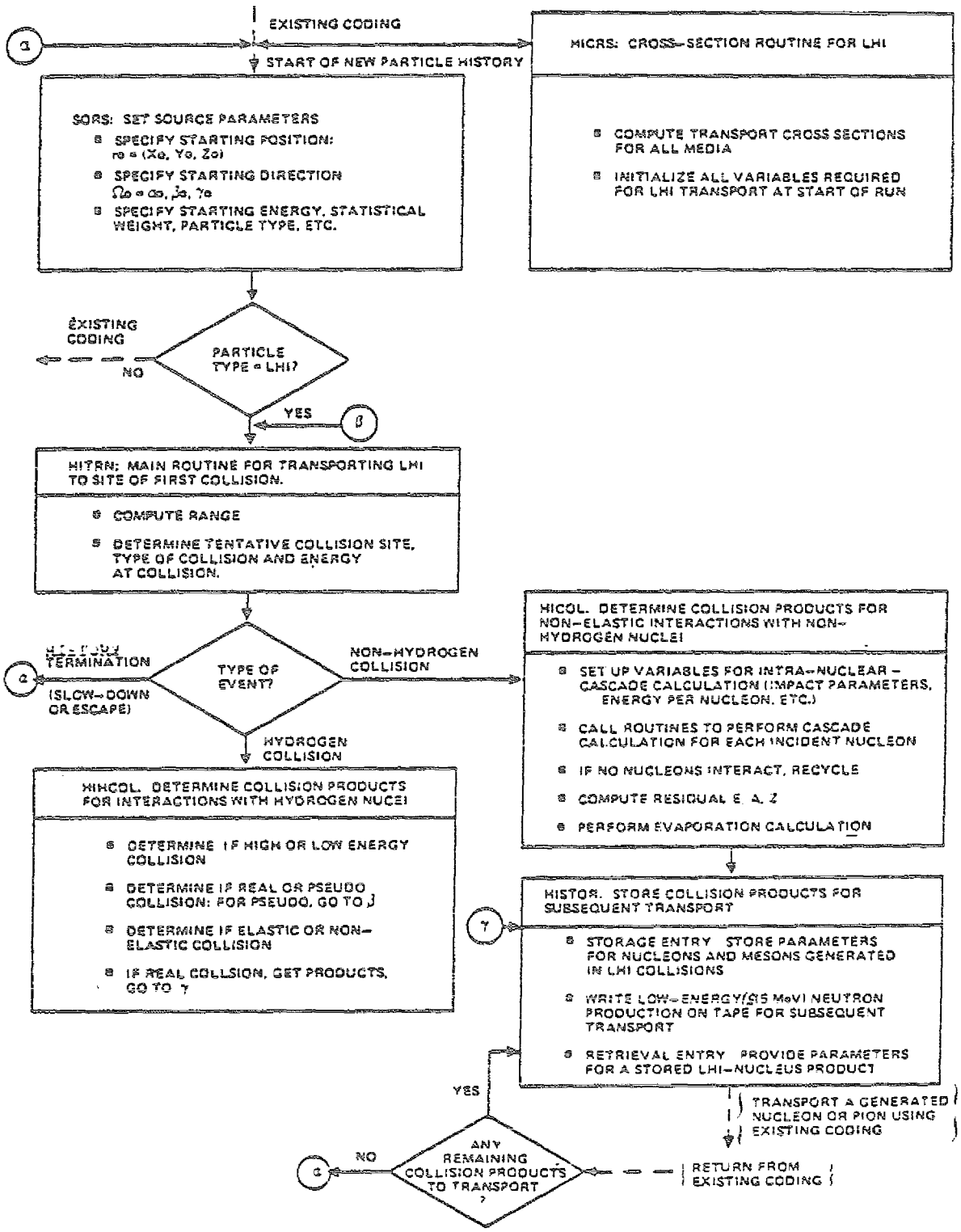

Fig. 8

New HETC subroutines for "light" heavy-ion (LHI) transport

Some results of calculations using this method are given in Ref. /15/ for a few cases: (a) neutron production for 160 MeV deuterons incident on thin targets of various materials, (b) energy deposition in a thick aluminum target for 1-GeV alpha particles, and (c) energy deposition in a thick U-238 target from 330 MeV deuterons. From these cases, the model appears to give reasonably good predictions, but it has not been extensively tested.

2.3 Model for Determinig Spallation-γ Ray Production and Transport

In the standard version of the HETC code the nuclear excitation remaining after a non-elastic collision (i.e., after the intranuclear cascade and the de-excitation by nuclear evaporation until particle emission is no longer energetically possible) is assumed to be dissipated by γ-ray emission. While the total γ energy, and the A and Z of the residual nucleus, is computed, the γ-ray spectrum is not available, so the transport of these γ-rays is not possible. There are several situations related to the SNQ in which the effects of such spallation γ-rays may be appreciable (e.g., heating in the cold source region, and in assessing the γ-ray background). Therefore, we have made modifications for the HETC/KFA-1 code to allow the effects of these spallation γ-rays to be computed.

The basic method is to: (a) output (optionally) on tape the residual A, Z, and remaining excitation energy for each collision which occurs during the high-energy radiation transport, (b) use this tape as input and apply a statistical model to compute, by Monte Carlo, the discrete γ-ray energies for each collision, and (c) store these γ-rays on a tape that can be used as an input source for a γ-ray transport code, such as MORSE. The model has not been throughly tested and should be regarded as preliminary at present.

2.3.1 Basic Theory Used

The application of statistical theory to predict γ-ray spectra from nuclear interactions is discussed by Troubetzkoy /16/, and this is basically the model coded here. (The approach of using this type of γ model in conjunction with the intranuclear-cascade-evaporation interaction model has previously been applied by Hill and Simpson /17/.)

The main assumption of the model is that all radiative transitions are of the electric dipole type. The transition probability from a state E to a state E' is broken into three parts:

$$S(E,E') = S_1 + S_2 + S_3$$

where S_1 refers to transitions within the continuum, S_2 refers to transitions from the continuum to a discrete level, and S_3 is for transitions between discrete levels. Within the continuum,

$$S_1(E,E') = \frac{f_1(E)\ (E-E')^3\ \rho(E')}{\sum_{i=0}^{n} (E-E_i)^3 + \int_{E_c}^{E} \rho(E')(E-E')^3 dE}$$

where f assures proper normalization of S, ρ is the continuum level density function (which is taken from Varshni /18/), and E_c is the lowest energy of the continuum. For a transition from within the continuum to a discrete level E_i,

$$S_2(E,E'_i) = \frac{f_2(E)\ (E-E_i)^3}{\sum_{i=0}^{n} (E-E_i)^3 + \int_{E_c}^{E} \rho(E')\ (E-E')^3 dE}$$

and between discrete levels,

$$S_3(E,E'_i) = \frac{f_3(E)\ (E-E'_i)^3}{\sum_{i=0}^{n} (E-E_i)^3}$$

For S_3, E is taken as the discrete level closest to the excitation energy.

2.3.2 Implementation

In the HETC/KFA-1 input, an option is provided to write an output tape for each nonelastic (non-hydrogen) collision containing information describing the A, Z, excitation energy, and spatial position of the residual nucleus. (The variable names written, by subroutine ANALYZ, are APR, ZPR, UU, XC(NO), YC(NO), ZC(NO), AND WT(NO).) An end-of-batch record is written with all variables set equal to -1.

A small code, called GAMA, reads these records and computes, on a collision-by-collision basis, the γ-ray energies. GAMA also reads a data base of nuclide energy levels, which were taken from /19/. GAMA writes a tape for each collision containing the γ-ray energy (in MeV), collision position (same as input), and the γ statistical weight. The record is EG,XC(NO), YC(NO), ZC(NO), AND WT(NO), with an end of batch record containing -1. for all variables.

The output tape from GAMA can be used as a source for the MORSE code to compute the γ-ray transport. The MSOUR(N) subroutine reads the input tape, defines the γ-ray energy group index IG, sets the starting position coordinates and weight, and sets N=-1 as an end-of-batch key. The MORSE main routine checks N as an end-of-batch signal rather than the usual procedure of counting source particles.

2.4 Miscellaneous Updates

2.4.1 Low-Energy Transport Cutoffs

An option has been added to allow different cutoff energies for ionization and nuclear collisions for charged particle transport. For protons the input parameter ELOP was used as the energy cutoff for both nuclear collisions and ionization. Now, EL is for nuclear collisions only, and a new input parameter, EPCUT, is used for the proton ionization energy cutoff. New input parameters, EPICUT and EMUCUT, have been added as cutoff energies for charged pions and muons, respectively. Thus, the ionization cutoffs are independent for different charged particles, whereas formerly the pion and muon cutoffs were fixed relative to the proton cutoff specified.

The EMIN array in labeled common /COMON/ now contains the ionization energy cutoffs for charged particles and the neutron collision cutoff. The collision cutoff for protons, ELOP, is now passed through the new common /ECUTP/.

2.4.2 Coulomb Scattering

In the versions of HETC distributed by RSIC there was a problem in that the Coulomb scattering subroutine SPRD did not properly update certain variables at material boundary crossings. This problem has been corrected with the Coulomb scattering routines incorporated in HETC/KFA-1. At present, these Coulomb scattering routines are compatible with general (or the cylindrical) geometry modules and are also interfaced with the combinatorial geometry package.

2.4.3 Range Straggling

In some applications involving low-energy charged particle sources in which the fraction of the beam particles that slow down and stop from ionization energy losses rather than undergo nuclear collision is significant, it is necessary to take into account the statistical fluctuations in energy loss. These fluctuations result in a variable range distribution (i.e., range "straggling"). In the standard version of HETC only mean ranges and average energy losses are computed. In HETC/KFA-1, energy-loss fluctuations and range straggling are incorporated for the primary beam particles.

The straggled range distribution is taken to be Gaussian about the mean range with a variance given by /20/:

$$\sigma^2_{iR}(E \Rightarrow E') = 4\pi e^4 Z^2_i n \int_{E'}^{E} \frac{(1-1/2\beta^2)\ K(E)}{(1-\beta^2)(1+(2m_e/m_i)\gamma)} (S_i(E))^{-3} dE$$

where $\sigma^2_{iR}(E \Rightarrow E')$ = the variance of the range distribution for a particle of type i slowing down from kinetic energy E to E',

e = the electron charge,
Z_i = the charge of the particle slowing down,
n = the electron density of the stopping medium,
K = the binding correction factor,
$\beta^2 = |(E^*+1)^2-1|/(E^*+1)^2$,
$E^* = E/m_i c^2$,
m_e = the electron mass,
$\gamma = (1-\beta^2)^{-1/2}$,
S_i = the stopping power.

The factor K takes into account the binding effect of the atomic electrons at low E.

Ranges are chosen from the distribution

$$p(R_i)dR_i = \frac{1}{\sigma^2_{iR}\sqrt{2\pi}} \exp-\left\{\frac{(R_i-R_i)^2}{2\sigma^2_{iR}}\right\}dR_i$$

where R_i is the mean range. The mean range and variance for protons as a function of energy for each medium in the system are computed. Values of R_i and σ^2_{iR} for other charged particles are obtained by scaling the stored proton values; i.e.,

$$\overline{R}_i(E_i) = (m_i/m_p)\ \overline{R}_p(E_i\ m_p/m_i)$$

and

$$\sigma^2_{iR}(E_i) = (m_i/m_p)\ \sigma^2_{ip}(E_i\ m_p/m_i).$$

If in the slowing down the particle passes from one material to another, a new straggled range is chosen based on the material being entered and the energy at the medium boundary.

Ranges are retrieved from subroutine RAINGE with arguments (ENG, MAT, ITYP, RNG). The "straggled" range corresponds to RNG, and the mean range at energy ENG corresponds to the variable RBAR contained in the labeled common /RNGAVG/. This common also contains the variance σ^2_{iR} as the variable SIGR.

3 INPUT DESCIPTION AND OPERATION OF HETC/KFA-1

3.1 Format of Primary Input

The primary input for HET-KFA consists of three sections:

Input section 1: Run header

- Card 1: FORMAT (14A4): Headline
- Card 2: FORMAT (14A4): SUBMIT - used as an identification for the history tape
- Card 3: FORMAT (3Z4) : RANDOM - hexadecimal start number for the random number generator (must be positiv and odd!)

Input section 2: includes all other input except the geometry description.
For the contents of Input section 2 refer to chapters 3.2 to 3.4. Input section 2 is read using FORTRAN NAMELIST-read

Syntax:

```
 &RUN assignment_1, assignment_2,...,assignment_I,
 assignment_1,...
 .
 .
 assignment_n
 &END
```

where assignment means:
variable name=constant
array name=const.$_1$,const$_2$,...,constant$_n$
array element=const.

where the constant may be integer
real
or literal
with respect to the type and length of the variable and array element is: array name (subscript list)
with unsigned integer constant subscripts

Rules:
- The first collumn of each card must be blank
- The sequence of assignments is arbitrary
- leading blanks may be used before assignments and constants to achiev better readability, but
- no trailing blanks are allowed after constants, because those are converted to zeroes.
- redundant data need not be assigned. For example: if you have two different materials, the hydrogen density for material index 3 to 15 need not be given.

Input section 3: includes the geometry description. This is formatted and depends on the geometry module linked in your job Refer to APPENDIX C.

3.2 Run Parameter and Model Options

Variable=default meaning

IHOUR=0	max. cpu-time allowed for this problem.
IMINIT=0	Since the timer is tested at the end of
ISEC=30	batch, this prediction should be somewhat less than the cpu-limit in the JCL The time limit is given in hours (IHOUR), minutes (IMINIT) and seconds (ISEC)
MAXBCH=2	The number of batches to be run with the present set of input data. The total number of source particles initiated with the present input will be MAXCAS*MAXBCH. For muon transport using a previously produced nucleon-pion history tape, both MAXCAS, and MAXBCH are calculated in subroutines MFPD; hence input values for these quantities are not used although they are written on the muon collision tape.
MAXCAS=2	no. of source particles per batch
EMIN(1)=15	energy of cutoff for proton
EMIN(2)=15	energy of cutoff for neutron
EPICUT=1	energy of cutoff for pion
EMUCUT=1	energy of cutoff for mueon

ELOP=15 The cutoff energy in MeV for proton nuclear collisions must be > 1 MeV)

CTOFE=0 not used

EMAX The maximum energy of particles being transported in MeV. For source muons EMAX is arbitrary. However, if source muon data are to be obtained from a previously produced nucleon-pion history tape, then by conservation of energy EMAX should not be less than $E_{\pi,max} + m_{\pi} - m_{\mu} = E_{\pi,max} + 33$ where $E_{\pi,max}$ is the value of EMAX which was input for the nucleon-pion calculation, m_{π} is the charged-pion rest mass, and m_{μ} is the muon rest mass. EMAX must be > ESR for nucleon-source.

ELAS=0 max. energy for neutron elastic collisions (100 MeV)

NEUTP=10 if not 0 & IBERTP<0 unit no. for low energy neutron tape
IBERTP>0 history tape of a previous run for mueon source
If nucleons and pions are to be transported, NEUTP is the logical number for the tape on which descriptions of neutrons appearing below ELON are written. IF NEUTP.LE.0, the low-energy neutron tape will not be written.
If the transport is for muons and source muons are to be obtained from a previously produced nucleon-pion tape, then NEUTP is the logical number of the nucleon-pion history tape.

NHSTP=30 if>0: unit number for the history tape

IGAMTP=0 if>0: unit number for the input tape of the γ generation code

IBERTP=-20 I-N-C and evaporation data tape
>0 for nucleon-pion-transport
=0 for mueon-pion-transport
<0 for nucleon-pion-mueon-transport

NELSTP=0 The logical number of the BCD tape containing the elastic scattering data for NOELAS nuclides. If NELSTP is the logical number of the standard input, the code expects all of the elastic scattering data to be input on cards after the primary input data and before the geometry input data.

N1COL=0	if>0: stop the history after the second generation useful for debugging I-N-C or generating XSECTIONS
NPIDK=1	if>0: π^- decay reaching their cut-off energy <0: π^- is forced to interact via I-N-C
NBOGUS=1	if>0: exitation of nuclei after INC is corrected with their recoil energy prior to evaporation
NSPRED=0	if>0: perform small angle multiple coulomb scattering for charged primary particles
NWSPRD=0	if>0: record small angle multiple coulomb scattering on the history tape
NSEUDO=1	if>0: record pseudo collisions (non productiv I-N-C) on the history tape NSEUDO should be > 0, when using a nucleon-pion run as source for a (pion)-muon run
ISTRAG=0	if>0: perform range straggling for charged particle ionisation
IANG=1	If IANG=0 secondary evaporation particles are produced isotropically in lab-system If IANG=1 secondary evaporation particles are produced non-isotropic (IANG must be=0 if fission is used).
IFISS=0	if>0: perform high energy fission during evaporation using the RAL fission model (prohibits IANG)
IBO=1	if>0: compute evaporation level density parameter according to A after each cluster evaporation step.
BO=8	if>0: overwrite the default BO of 8 MeV in EVAP and RAL fission model
IGEOM=0	0: combinatorial geometry used 1: general geometry used -1: cylindrical geometry used the corresponding module must be linked
NLEDIT=0	if>0: print an edit of the elastic neutron collision x-section if used
NOELAS=0	number of elements for which neutron elastic x-sections are to be read
LHI=0	switch for heavy ion beams 1 d 2 t 3 He^3 4 α 5 arbitrary heavy ion

HIA(5)=0 mass of an arbitrary heavy ion
HIBE(5)=0 binding energy of an arbitrary heavy ion
HIZ(5)=0 charge of an arbitrary heavy ion

3.3 Material Composition

MXMAT number of different media exclusiv voids (must be >0 and <16)
NEL(j) number of elements other than hydrogen of material j,j = 1, MXMAT must be < 10 for all materials
NOEL(j) number of elements with elastic neutron scattering other than hydrogen of material j, j = 1, MXMAT must be < NEL(j)
DENH(j) hydrogen density in material j, j=1, MXMAT
A(i,j) A(i,j)is the mass number of element i=1, NEL(j) in material j=1, MXMAT
ZZ(i,j) ZZ(i,j) is the charge number of element i=1, NEL(j) in material j=1, MXMAT
DEN(i,j) DEN(i,j) is the nuclear density of element i=1, NEL(j) in material j=1, MXMAT
MEDEQ(j) medium equivalence information to be used with general geom (will be set automatically)
ID(i,j) identification (sequence number) of the neutron elastic scattering data for element i, i=1, NOEL(J) in material j, j=1 MXMAT

3.4 Source Particle Description

XSR=0
YSR=0 position of the source particle
ZSR=0

ESR energy of the source particle

USR=0
VSR=0 direction cosines of the source particle
WSR=0 (if all are zero isotropic distribution is assumed)

XSIG=0
YSIG=0 standard deviation of the source particle's position
ZSIG=0 (each coordinate sampled from a gaussian distribution)

ESIG=0 standard deviation of the source particle's energy (sample E from a gaussian distribution)

RSR=0 truncation radius for $X^2 + Y^2 < RSR$ with X = XSR + Gauss. (XSIG), Y = YSR + Gauss. (YSIG)

TIPSR=0

0	proton source
1	neutron source
2	π+ source
3	π0 source (forbidden)
4	π- source
5	μ+ source
6	μ- source
7	d for LHI=1
8	t for LHI=2
9	He^3 for LHI=3
10	α for LHI=4
11	heavy ion for LHI=5

WTSR=1 statistical weight of source particle

4 GENERAL-PURPOSE ANALYSIS CODE SIMPEL

4.1 General Features

SIMPEL originally has been developed in connection with the feasibility study for the german spallation neutron source SNQ.

The code provides a tool for the statistical analysis of simulated particle cascades. The first release of the code completely relies on the high-energy-transport code HETC.

HETC generates a so-called history tape, containing information about the particles which have been transported through an arbitrarily specified 3D geometry with up to 15 different materials in it.

The events recorded on the tape are:
- generation of incident particles
- spallations
- ionization-energy losses of charged particles down to a specified cut-off energy
- escapes of particles from the geometry
- boundary crossing of particles from one material zone to another
- decays of π-ons
- elastic neutron scatterings
- small-angle coulomb scatterings of charged particles

There is additional information on the tape,
- start of run
- start of batch
- end of batch
- end of run

where a 'run' is a number of several 'batches', and a 'batch' is a number of several 'histories'. A 'history' consists of all of the information (contained in records) related to one incident particle.

For each event the following information is avaialble:
- xyz,uvw,e : the phase space coordinates of the particle at the collision site of the current collision, and for the previous collision

- wt,tip : the statistical weight and the type of the particle
- z,a : charge and mass number of the struck nucleus (after collision)
- ex,erec : excitation and kinetic energies of the struck nucleus (after collision)
- phase space coordinates,statistical weights and types of secondary particles (from intra-nuclear cascades and evaporation)

SIMPEL scans the HETC-history tape event by event summing up the contributions of the event to physical properties of interest. (such as track lengths or energy deposition) At the end of each batch SIMPEL computes the batch-mean-values of the sampled data; at the end of run the batch-mean-values are reduced to run-mean-values and their fractional standard deviations.

There are several detector types defined in SIMPEL, which the user can select on input to get information of

- particle flux and current
- the yield and distribution of secondary particles from intranuclear cascades and evaporation
- the distribution of residual nuclei
- energy deposition

The detectors may be set up to provide their results in

- energy bins (for flux,current and secondary particle distribution)
- angle bins (for flux,current and secondary particle distribution)
- space regions
- mass and charge (for residual nuclei)
- particle type (one single particle type is assigned to the detector)
- contribution type (for energy-deposition detectors)

If resolution in bins is selected, the user may request automatic normalization to the bin width.

Since SIMPEL was intended to be a general-purpose-analysis code, it was designed in a way, that it can easily be extended. Thus, a modular program structure was used. Most of the statistical routines do not consider the

type of detectors used. Installing a new detector type simply means to extend the detector-definition routine, the scoring routine and the result-printing routine. Even if we want to run SIMPEL with other types of history-tapes, only an appropriate data interface has to be written. It is also possible to run SIMPEL as an incore-analysis program by installing a monte carlo code as a SIMPEL module. The only restriction would then be, that the monte carlo code must not violate the core management of SIMPEL, i.e. it should not use the blank common without asking for a reservation of blank common by the SIMPEL driver COMSYS.

It is actually planned to extend SIMPEL to provide more detectors and to allow more powerfull data manipulation.

4.2 Description of Simpel Program Modules

SIMPEL consists of several modules, supervised by the driver module called COMSYS.

COMSYS
- reads the command input,
- controls allocation of data in blank common,
- controls execution of the other modules according to the command input
- provides service routines for data input and presentation

The executive modules are:

HETANA
- which defines and performs the analysis of a HETC-history tape
  (see chapter 4.4)

STATIST
- providing routines for binning, normalization and variance analysis

CG-GEOM
- which defines and performs geometry tasks.
  (see APPENDIX C)

PICTURE
- which tests the geometry definition.
  (see APPENDIX D)

4.3 Input Description

To run SIMPEL two input sources are necessary:

- one or more HETC-history tapes,
- the command input.

The latter one is used to specify the geometry, the detectors to be used, and the binning applied with the detectors. Thus, the command input normally consists of

- the GEOIN command,which reads the combinatorial geometry description used in the analysis,
  This may provide a more detailed resolution than the original HETC-geometry description.
  If no geometry description is used, SIMPEL will use the HETC media to resolve space.
- the PICTURE command,if the user wants to test his geometry input,
- several ASSIGNMENT statements or VECTOR commands,to define FORTRAN-like arrays and fill them with input data.
  Such arrays are used for energy- or angle-group limits, volumes or surface-areas for normalization, lists of region numbers to be looked at in a detector and so on.
- several DEFDET commands, which define the types of analysis to be performed and to connect the detectors with the binning and geometry information. (i.e. you request special bin-arrays, region number lists for the detector, you specify the type of particle to be looked for and the type of physical property you want to sample)
- a SIMPEL command for each HETC-run to be analyzed.

Additionally there may be commands to save or present special portions of data.A STOP command will at last terminate the analysis.

In the following you will find the description of the syntax and function of the available commands.

--> General command syntax

A command consists of the command name and up to 15 parameters. The parameters are separated by commas. The command is terminated by a semi-colon ';'. Each parameter may be

specified either positional or by keyword.
Consider 'COMNAME' the name of a command with three parameters named 'PARM1','PARM2', and 'PARM3',
then COMNAME PARM1=$value_1$,PARM2=$vaule_2$,PARM3=$value_3$;
and COMNAME $value_1$,$value_2$,$value_3$;
will be equivalent.

Omitting parameters will cause the program to provide some default values ,or if no default is available to print an error message.
Thus COMNAME PARM3=$value_3$;
will cause 'PARM1' and 'PARM2' to be defaulted;
dto. COMNAME ,,$value_3$;
where position-holding commas are used to replace the missing parameters. In any case the sequence of parameters must not be changed;
i.e. COMNAME ,,$value_3$,PARM2=$value_2$;
is invalid, because 'PARM2' must preceed 'PARM3'.

The value assigned to a parameter may be:

- an integer or real constant,
- an integer or real vector (i.e. a list of constants separated by commas or blanks and enclosed in parenthesis),
- a text string enclosed in quotes (i.e. 'text')
- the variable name of a predefined item or array
- a variable name of an item or array which is to be defined by the command's executive routine.

For each parameter a well defined type of value is requested. (see commamd KEY)

--> Assignment statement

The assignment statement is used to assign integer or real constants or arrays to a variable name. These names may be used in subsequent commands.

Examples:
- I=14;
- PI=3.1415;
- INDEX=(1,3,5,7);
- ANGLE=(0. 15.0E0 30. 40.);

Variable names may consist of up to six characters. The data type of a variable is determined by the type of constant being assigned (not by FORTRAN name conventions !).

--> ASCCOM-command

function: printout all command names available in this release of SIMPEL.
syntax : ASCCOM;
remarks : ASCCOM will be helpful, when running SIMPEL in an interactive operating system.

--> ASCNAM-command

function: printout all user-defined variable names
syntax : ASCNAM;
remarks : ASCNAM will be helpful, when running SIMPEL in an interactive operating system.

--> KEY-command

function: printout the names and data types of all parameters of the command specified.
syntax : KEY NAME=command_name;
(no default)

remarks : KEY will be helpful, when running SIMPEL in an interactive operating system.
The output will include

command-name $parm_1$ $type_1$ $parm_2$ $type_2$
$parm_3$ $type_3$ $parm_4$ $type_4$
...
...

where $parm_i$ is the parameter-name
and $type_i$ is the parameter-type with
$type_i$= 3 variable name to be used in the executive routine
4 for integer item
5 for real item
6 for text item
7 for integer array
8 for real array

(Data types 1 and 2 are reserved for command-names and parameter names respectively.)

--> DELETE-command

function: delete an array entry (variable) from the list of user defined variables.
If possible, the blank-common area where it has been allocated is freed.

syntax : DELETE NAME=variable name;
(no defaults)

remarks : -/-

--> PRINT-command

function: printout of the contents of a user defined variable in standard format.

syntax : PRINT NAME=variale name,
IOUT=output unit #;
(default:IOUT=6)

remarks : -/-

--> GEOIN command

function: read in the description of the geometry according to CG-input conventions from a specified unit and print out the control information provided by the CG routines.

syntax : GEOIN IN=input unit #,
IO=output unit #;

(default: IN=5,IO=6)

remarks : Refer to APPENDIX C for input desciption of the CG routines.
The user may as well link another geometry code with SIMPEL, which has the same interface.

--> PICTURE-command

function: line printer plots will be made on unit IOUT showing cross sections through the geometry described by means of the GEOIN command. Location and orientation of the planes are read from unit IN.

syntax : PICTURE IN=input unit #,
IO=output unit #;
(defaults: IN=5,IO=6)

remarks: For definition of the planes by input refer to APPENDIX D
PICTURE will run with any geometry code, having the CG interface.

--> VECTOR-command

function: defines a variable as an array entry and reads in data in free format.

syntax : 1. VECTOR NAME= variable name,
LEN= array length,
TYP= 0:integer / 1:real,
PRINT= 0:no print/ 1:print;
2. LEN real or integer constants (according to TYP) separated by blank or comma (where two commas replace a zero).
3. the list of constants is terminated by ; or T
(defaults: TYP=1,PRINT=0)

remarks : -/-

--> MATRIX-command

function: defines a variable as two-dimensional array entry and reads in data in free format.

syntax : 1. MATRIX NAME= variable name,
VECNO= number of vectors forming the martrix,
VECLEN=length of these vectors,
TYP= 0:integer / 1:real,
PRINT= 1:printout as read /
0:no print,
TRANS= 0:store vectors as lines /
1:store vectors as columns;
2. VECNO list of constants (vectors) each consisting of VECLEN constants of type TYP separated by blank or comma.
3. each list of constants is terminated by; or T
(default: TYP=1,PRINT=0,TRANS=0)

remarks : -/-

--> STOP-command

function: terminates execution of SIMPEL
syntax : STOP;

remarks : must allways be last command on input.

--> SIMPEL-command

function: performs the analysis of a HETC-history tape
using the geometry specified by GEOIN,
all detectors specified by DEFDET.
syntax : SIMPEL NHSTP= unit # for history tape,
NBAT= number of batches to be ana-
lyzed,
IOUT= output unit #
INCLUD= list of HETC media to be scored,
EXCLUD= list of HETC media to be excluded
from scoring;
(defaults: IOUT=1)

remarks : INCLUD and EXCLUD are optional but must not be
used at the same time. They preselect events
for the analysis process. Thus using INCLUD or
EXCLUD will reduce the CPU time requirements of
SIMPEL. Make sure that no media are excluded from
analysis which lie whithin a detector region.

If no GEOIN command has been used, SIMPEL will
use the HETC media numbers as region numbers.

--> DEFDET-command

function: defines a detector for the analysis.
(see also chapter : "Methods of analysis")

syntax : DEFDET NAME= first 4 characters of the names
of arrays to be defined,

TYP= detector type (see table DETECTORS),
IOPT= (not used),
IPRT= particle type (see table PARTICLES),
W= detector-reference direction
given as (u,v,w),

NORM= normalization request given as (n_e,n_η,n_v) where n_i=1 turns normalization on,
n_e=1 -- per ΔE
n_η=1 -- per solid angle
n_v=1 -- per space-unit as input in VOL (see table DETECTORS)

MARG= request for marginal responses given as (m_e,m_η,m_r,$m_{e\eta}$,m_{er},$m_{\eta r}$) where m_i=1 turns margin on, (see table DETECTORS)

E= name of energy-bin vector, (for residual nuclei detectors, E contains a list of nuclei ZZ.AAA)

A= name of η-bin vector where η is the angle between W and the flight direction,

R1= name of the list of region numbers of interest.

R2= name of the list of region numbers, if given,the surfaces between R1 and R2 are detector surfaces of interest,

VOL= name of volume or area vector for normalization to space or surface units;

one card of text as headline for the detector output

(defaults: TYP=2,IOPT=0,IPRT=1,W=(1.,0.,0.), NORM=(0,0,0),MARG=(0,0,0,0,0,0))

--> table : DETECTORS

ITYPE	calculated property	
1	$Y(E,\eta,R)$	number of secondary cascade particles produced in energy bins E and angle bins η and regions R.
2	$Y(E,\eta,R)$	number of secondary evaporation particles produced in energy bins E, angle bins η and regions R.
3	Y(z.a,,R)	number of residual nuclei with charge z and mass a in regions R.
4	$\Phi(E,\eta,S)$	fluxes of particle IPRT through surfaces S in energy bins E and angle bins η .
5	$J(E,\eta,S)$	current of particle IPRT through surfaces S in energy bins E and angle bins η .
6	dE(typ,R)	energy deposited in regions R by primary protons, secondary protons, energy of neutrons prduced below energy cutoff, charged π and μ-ons, heavy ions, nucleus excitation, π^0, all secondary part. and total dE
7	$\Phi(E,\eta,R)$	fluxes of particle IPRT in regions R in energy bins E in angle bins η

ITYPE	Normalizations			Margins					
1	n_E	n_η	n_R	Y(R)	Y(η)	Y(R)	Y(E,η)	Y(η,R)	Y(E,R)
2	n_E	n_η	n_R	Y(R)	Y(η)	Y(R)	Y(E,η)	Y(η,R)	Y(E,R)
3	-	-	n_R	Y(nuc)	-	Y(R)	-	-	-
4	n_E	n_η	n_S	Φ(E)	$\Phi(\eta)$	Φ(S)	Φ(E,η)	$\Phi(\eta$,S)	Φ(E,S)
5	n_E	n_η	n_S	J(E)	J(η)	J(S)	J(E,η)	J(η,S)	J(E,S)
6	-	-	n_R	dE(typ)	-	dE(R)	-	-	-
7	n_E	n_η	n_R	Φ(E)	$\Phi(\eta)$	Φ(R)	Φ(E,η)	$\Phi(\eta$,R)	Φ(E,R)

--> table : PARTICLES

particle	number (IPRT)
primary part.	1
secondary p	2
secondary n	3
π^+	4
$\pi 0$	5
π^-	6
μ^+	7
μ^-	8
deuteron	9
triton	10
he^3	11
α	12
not-used	13
not-used	14
π (total)	15
μ (total)	16

4.4 Methods of Analysis

The analysis of a HETC-history tape is performed by the module HETANA which consist of the subroutines

- SIMPEL which reads the tape, and calls the other analysis routines according to the type of event record found.
- SCOR computes the result contribution 'x' of an event to each defined detector,
  finds the correct bin number for angle and energy using the functions IUPS and IDOWNS ,
  finds the matching region or surface numbers by the means of LOOKZ and GEOM,
  and accumulates 'x' into the batch-result array of the detector
  $X_{det.} = X_{det.} + x$
- EBATCH picks up 'X' at the end of each batch and computes
  $X_{det.} = X_{det.} / nsour$,
  where 'nsour' is the number of source-particle in the current batch.

Thus X is converted to the mean value of the detector response; i.e. total response per source particle in the last batch.

Then EBATCH computes

$M_{det.} = M_{det.} + X_{det.}$ and

$S_{det.} = S_{det.} + X_{det.}^2$

- ERUN is called at the end of the analysis.
It computes the mean of X over all batches and stores it in the M array

$M_{det.} = M_{det.} / nbatch$

Then it computes the percent error of M

$S_{det.} = (S_{det.} - M_{det.}^2) / (nbatch-1)$

$S_{det.} = S_{det.} * 100. / M_{det.}$

by calling VAR1 for each detector

If desired ERUN performs also normalization to unit energy, solid angle and region volume or surface area.

Finally OUT2 is called for each result array to print the results on the desired unit.

If the user requested marginal distributions for a detector, then additional M and S arrays are available for this detector and EBATCH will reduce $X_{det.}$ to $X_{marg.}$ and add

$$S_{marg.} = S_{marg.} + X_{marg.}^2$$

and ERUN will reduce $M_{det.}$ to $M_{marg.}$ and convert $S_{marg.}$ to the percent error of $M_{marg.}$

The core of the analysis modules are the routines SCOR1 and SCOR2. These routines share the task of computing event contributions 'x' for the detectors specified.

SCOR1 is used for contributions which arise at the point of a physical event.

It consists of a loop over all detectors defined in input

Detector	Process
1 $Y(E,\eta,R)$	it scans all secondary particles coming from INC process, - checks the particle type - finds energy bin I_E of the particle - finds angle bin I_η of the angle η between the flight direction $\vec{f}$ and the detector's reference direction $\vec{d} = (u_{det.}, v_{det.}, w_{det.})$ - finds the region bin I_R by calling LOOKZ - and computes $X(I_E, I_\eta, I_R) = X(I_E, I_\eta, I_R) + WT$ where WT is the statistical weight of the particle. - particle types allowed are protons, neutrons, pions and muons.
R_2 $Y(E,\eta,R)$	it scans all secondary particles comming from evaporation of the struck nucleus, - finds I_E, I_R and I_η as above - and computes $X(I_E, I_\eta, I_R) = X(I_E, I_\eta, I_R) + WT$ - particle types allowed are protons, neutrons, deuterons, tritons, He^3, and alphas.
3 $Y(A.Z,R)$	it looks for the index I_{nuclid} of the residual nucleus using A and Z and finds I_R as above. Then it computes $X(I_{nuclid}, 1, I_R) = X(I_{nuclid}, 1, I_R) + WT$ where WT is the weight of the incoming particle.

(continue on next page!)

6 dE(type,R) it finds I_R by calling LOOKZ and computes the energy deposited by

- heavy ions (including the struck nucleus the range of which is supposed to be very short)
  $E_d * WT_d$
  $E_t * WT_t$
  $E_{He3} * WT_{He3}$
  $E_\alpha * WT_\alpha$
  $E_{nucleus} * WT_{incident\ particle}$ (where E is the recoil energy)

- secondary π^0's (which are supposed to decay prompt)
  $(E_{kinetic}+E_{restmass}) * WT_{\pi 0}$

- particles reaching their cut-off energy or generated below their cut-off energy
  $E_p * WT_p$
  $E_n * WT_n$ (not included in total dE)
  $(E_{\pi-}-1.) * WT_{\pi-}$ (1 mev for binding)
  $E_{\pi+} * WT_{\pi+}$
  $(E_{\mu+}+106.) / 106. * 33.328 * WT_{\mu+}$
  $((E_{\mu-}+106.) / 106. * 33.328 - .511 * WT_{\mu-}$
  for μ's part of the energy will be lost in flight.
  for μ^- electron restmass is subtracted

The contributions are stored
$X(I_{type},1,I_R) = X(I_{type},1,I_R) + con$

SCOR2 computes contributions arising in flight. Thus, SCOR2 has to divide the path of a particle corresponding to the spatial bins defined by the CG-GEOM routines.

Therefore SCOR2 is organized in two loops:
The outer loop starts calling LOOKZ to find the region number of the starting point of the path. Then GEOM is called to find the length of the first sub-path (to the next boundary or to the collision point). For each sub-path SCOR2 runs the inner loop over all detectors defined and performs:

Detector	Process
4 $\Phi(E,\eta,S)$	the flux contribution of a particle of type IPRT through a surface I_S which is specified by the two region numbers sharing S , the angle bin I_η and the energy bin I_E. The contribution is computed as $con = WT_{prt.} / abs(\vec{n} * \vec{f})$ where $\vec{n}$ is the normal vector on the crossed surface at the crossing point and $\vec{f}$ is the particle flight direction. To find the energy bins I_E of charged particles, E has to be computed at the boundary. This is done using subroutine ECCOR which uses energy-range tables read from the HETC-history tape. ECCOR takes into account, that ranges may be straggled. It computes dE using mean ranges and scales by the ratio of unstraggled flight length to recorded flight. The result is stored by $X(I_E,I_\eta,I_S) = X(I_E,I_\eta,I_S) + con$
5 $J(E,\eta,S)$	the current contribution of a particle of type IPRT. This detector works like detector type 4. Only the contribution is taken as $con = WT_{prt.}$

(continue on next page!)

6 dE (type,R) the ionization-energy loss of charged particles. I_R is the region index of the current sub-path. The contribution is computed as

con = $(E_1 - E_2) * WT_{prt}$.

where E_1 is the particle energy at the starting point of the current sub-path.

and E_2 is the particle energy at the end of the current sub-path as computed by ECCOR.

7 $\Phi(E,\eta,R)$ the flux contribution of a particle of type IPRT in energy bins I_E,
angle bin I_η,
regions I_R
The contribution is computed as

con = PTH * WT_{prt}.

where PTH is the length of the sub-path for neutrons

or PTH is the length of the sub-sub-path for charged particles.

(Since charged particles lose energy approximately continuously by ionization, the sub-path has to be split once more into pieces where the particle's energy lies within one single energy bin. Thus an additional contribution loop is installed, to get the sub-sub-path using function RBAR and scaling the range with the straggling factor RB TO RS.)

5 MODIFICATIONS TO MORSE-CG

5.1 Coupling with HETC

Random walk and analysis of low energy neutrons generated by HETC cascades is done by MORSE. These neutrons are transferred to MORSE by their parameters: name (sequence number), energy in eV, direction cosine, location and weight, which are written on tape by HETC.

The number of neutrons varies from batch to batch, whereas MORSE processes in a given number of batches a fixed number of particles only. Thus a standalone routine selects a fixed number of neutrons for each batch and creates an input tape for MORSE, containing the characteristic parameters mentioned above.

To get valid representation, these N neutrons n_i are selected randomly from M neutrons, generated in a single HETC batch,using random numbers r_i (in the interval (0,1)):

$$n_i = r_i * M + 0.9999 \quad i = 1,N$$

At the end of analysis the fluxes calculated in MORSE are multiplied by the average number of neutrons NPS generated per source particle.

$$NPS = \frac{1}{N_s} * \sum_{i=1}^{M_t} WT_i$$

N_s - total number of HETC source particles
M_t - total number of neutrons in all HETC batches
WT_i- statistical weight of neutron i

5.2 Additional Estimation Routines in MORSE

Besides the well known SAMBO package we are using some additional estimation routines which are very helpful for flux and current estimation on surfaces. Flux and current are always estimated according to the well known equations:

$$\Phi(E) = \frac{NPS}{N*B} * \sum WT_i * COS_i$$

$$j(E) = \frac{NPS}{N*B} * \sum WT_i$$

B - number of batches stated in one run in MORSE-CG
WT_i - weight of neutron crossing the surface
COS_i - $=\mu_i * n$, direction cosine of neutron crossing the surface

a) Neutron flux and current on a plane surface between two regions A and B are estimated in a way, that only particles passing the surface from side A to B are detected. Energy dependent fluxes and currents and total responses are not normalized to the surface erea.

b) Neutron flux and current per cm^2 on a plane surface between two regions are estimated using a mesh net given in x-y coordinates over the defined surface between two regions. For each mesh flux and current per cm^2 and their fractional standard deviations are calculated. In case of a three-dimensional surface like a cylindrical surface, this detector cannot distinguish between top and bottom, only plane surfaces are possible.

c) Additional to flux and current per cm^2 maximum distributions are calculated for plane surfaces. These are not normalized to the mesh.

6 PERFORMANCE SCHEME OF THE KFA/IRE-1 CODE SYSTEM

To simulate the transport of nuclear particles in 3-dimensional assemblies the above described codes and auxiliary programs were implemented on IBM-3033. The currently used code system for spallation source calculations is shown in Fig. 9 as a block diagram. The experimental nucleon-nucleon and nucleon-meson cross sections and evaporation parameters are discussed in APPENDIX A and APPENDIX B. For the MORSE calculations several neutron and coupled neutron-γ libraries are in use: The EPR library /21/ (100 neutron groups, 10^{-4} eV to 14.9 MeV and 21 γ groups, 10^{4} MeV to 14 MeV); the HELLO library /22/ (35 neutron groups, 10^{-4} eV to 60.0 MeV, 21 γ-groups, 10^{-2} MeV to 14.0 MeV), the HILO library /23/ (66 neutron groups, 10^{-4} eV to 400.0 MeV, 21 γ-groups, 10^{-2} MeV to 14.0 MeV) and the LASL library /24/ (41 neutron groups, 1.39 10^{-4} eV to 800 MeV).

A special library for thermal neutron transport SPALIB with 53 neutron groups, 10^{-5} eV to 14.9 MeV with 26 groups below 1 eV including upscattering data, for target-moderator-reflector thermal neutron transport was derived from ENDF/B-IV by using the reactor code system RSYST /25/. Activation, energy deposition, special reaction cross-sections and kerma factors are generated via the MACK code /26/, the MACK-IV library /27/ or using the AMPX code /28/. A sample problem is demonstrated in APPENDIX E.

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APPENDIX A

Description of Input Data Used by the Evaporarion Model in the HET Code

A.1 Introduction

As part of the theoretical work on target physics related to the German spallation neutron study, the present calculational models and computer codes available for the prediction of high-energy radiation transport and effects are being reviewed. In particular, the accuracy of the nuclear interaction model (the intranuclear-cascade-evaporation model) employed by the radiation transport code HETC /A.1/ is being assessed by a series of comparisons with experimental data, and improvements (both in terms of updated input data and model modifications) are planned. In preparation for updating the input data used by the evaporation model, a detailed description (not presently available) of the data now used is given here. To help define the input data, some of the theory and historical background is also discussed.

The basic evaporation model theory used in the HETC code is that of Weisskopf /A.2/, with much of the method of implementation based in the work of Dostrovsky, et.al., /A.3-A.5/. The evaporation model used in HETC is an evolution of an evaporation code called EVAP, originally written by Dresner /A.6/ with a series of revisions by Guthrie /A.7,A.8/; the nature of these revisions are indicated in Table A.1.

These "stand-alone" EVAP codes have been incorporated as subroutines (and used in conjunction with the cascade model) to treat high-energy nuclear collisions in the thick-target radiation transport code HETC, and its predecessors NMTC and NTC, as indicated in Table A.2. Various updates have been made for the nuclear mass data used, and this is also indicated in Table A.2.

The evaporation data input described in this paper corresponds to that used by EVAP-4, which is the form of the evaporation model used in the version of HETC distributed by the Radiation Shielding Information Center (RSIC).

TABLE A.1

Basic Differences in EVAP Series of Evaporation Model Codes

Evaporation Code	Comments
1 EVAP /A.6/	original code
2 EVAP-2 /A.7/	only 6 types of evaporated particles considered instead of 19 in EVAP updated nuclear masses allows ^{8}Be as a residual nucleus to split immediately into two α particles recycles (up to a max of 10 times) if get kinetic energy selected greater than allowed by excitation energy
3 EVAP-3 /A.7/	like EVAP-2 except effects of kinetic energies of recoil nuclei taken into account
4 EVAP-4 /A.8/	identical to EVAP-3 except for "improved-termination" scheme for particle emission

A.2 Comments on Calculational Method

Some of the input data for the evaporation model consists of pre-computed functions which are used in various steps of the calculation. To define the meaning of these, and other input data, we briefly summarize here some of the steps of the evaporation calculation.

The probability $p_i(E)$ that a nucleus excited to energy U will emit a particle of type i having kinetic energy E is assumed to be expressed as

$$P_i(E) \propto g_i m_i E \sigma_{ci}(E) \omega(E^*), \qquad (A.1)$$

where g_i is the number of spin states, m_i is the emitted particle mass, σ_{ci} is the inverse cross section (i.e., the compound nucleus formation cross section corresponding to bombarding the residual nucleus with particles of type i and energy E), E^* is the excitation energy of the residual nucleus (E^*= U-Q-E, where Q is the binding energy of particle i), and ω is the density of energy levels of the residual nucleus.

The form for ω used is

$$\omega\ (E^*) \propto \exp\left\{2\left[a(E^*-\delta)\right]^{1/2}\right\} \qquad (A.2)$$

where δ is the pairing energy and

$$a=A/B_0(1+Y\Delta^2/A^2),$$

with A=mass number, B_0=8 MeV, Y=1.5, Δ=A-2Z, and Z=charge number. (Since Eqs. (A.1) and (A.2) are always involved in ratios in the computations, constants have been omitted.)

TABLE A.2

Overview of Nuclear Data Input Used in the EVAP Series of Evaporation Model Codes

Evaporation Code	Transport Code Used In	Nuclear Mass Data Used
1 EVAP	NTC /A.9/	(a) from tables compiled by Wapstra (1955) /A.11/ and Huizenga (1955) /A.12/ for bases where measured masses exist (b) semi-empirical formula of Cameron (1957) /A.13/ for nuclei not measured
2 EVAP-2 and EVAP-3	NMTC /A.10/	(a) Mattauch, et.al. (1965) /A.14/ tabulation of binding energies (b) Cameron semi-empirical mass formula /A.13/ for nuclei not tabulated by Mattauch et.al. (c) "shell-plus-pairing" energy corrections for Z or N < 13 from Peele and Aebersold /A.15/ rather than from Cameron
3 EVAP-4	HETC /A.1/ (RSIC Version)	same nuclear data as EVAP-2 and EVAP-3
4 EVAP-4' /unpublished/	HETC (some versions)	updated nuclear masses from Wapstra and Gove (1971) /A.16/

The inverse cross section is taken to be the geometric cross section modified by an empirical expression to take into account energy dependence, and a Coulomb barrier correction for charged particle emission. For neutrons,

$$\sigma_{cn}(E)=\pi R^2\alpha(1+\beta/\alpha) \qquad (A.3.1)$$

$$\alpha=0.76+1.93A^{-1/3} \qquad (A.3.2)$$

$$\alpha\beta=1.66A^{-2/3}-0.05 \qquad (A.3.3)$$

$$R=1.7A^{1/3} \qquad (A.3.4)$$

with R in units of fermions ($1fm=10^{-13}$ cm).
For charged particle emission,

$$\sigma_{ci}(E)=\pi R^2(1+C_i)(1-k_iV_i/E),$$

for $E>k_iV_i$, and zero otherwise. Here V_i is the Coulomb barrier calculated from the classical electrostatic expression and the factor k_i is inserted to take into account in an approximate way barrier penetration effects. The numerical values used for C_i and k_i are mainly those chosen by Dostrovsky, et.al. /A.4/ to give a good fit to continuum-theory cross sections. Values for protons and alpha particles are given in Table A.3, and the others are determined from the following relations:

$$k_d=k_p+0.06 \quad C_d=C_p/2$$

$$k_{H_3}=k_p+0.12 \quad C_{H_3}=C_p/3$$

$$k_{He_3}=k_\alpha-0.06 \quad C_{He_3}=C_\alpha=0$$

The expression used for Coulomb barrier is

$$V_i=Z_iZe^2/(R+R_i) \qquad (A.4)$$

where e is the electron charge and R_i is zero for protons and 1.2 fm for all other particle types.

TABLE A.3

Parameters Used for Computing Inverse Charged-Particle Cross Sections

Z	k_p	C_p	k_α
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

The first step in computing particle emission from an initial nucleus having A, Z, and U is to determine the total (over all energy) emission probability for each particle type which is

$$P_i=\hat{P}_i/(\sum_{i=A}^{6}\hat{P}_i), \text{ with}$$

$$\hat{P}_i=g_i m_i \int E\sigma_{ci}(E)\omega(U-Qi-\delta-E)dE$$

where the upper limit of the integration is $U-Q_i-\delta$ and the lower limit is k_iV_i. (This equation is applicable, of course, only if emission is energetically possible -- i.e., if $U>k_iV_i+Q_i+\delta$. Otherwise, $P_i=0$).

Based on the work of Dostrovsky, et.al. /A.3/, this integral is performed analytically. The result (within a common numerical factor) is:

for neutrons,

$$\hat{P}_i=A^{2/3}\alpha(I_1(S)+\beta I_0(S))e^S, \qquad (A.5.1)$$

and for charged particles,

$$\hat{P}_i=(g_i m_i/2)(1+C_i)A^{2/3}I_1(S)e^S \qquad (A.5.2)$$

where

$$S=2(a(U-k_iv_i-Q_i-\delta))^{1/2} \qquad (A.5.3)$$

$$I_0(S)=(2a)^{-1}(S-1+e^{-S}) \qquad (A.5.4)$$

$$I_1(S)=(8a^2)^{-1}(2S^2-6S+6+e^{-S}(S^2-6)) \qquad (A.5.5)$$

The kinetic energy selection for the evaporated particle is based on the equation

$$N(E_i)dE_i=T_2^{-2}W_i\exp(-W_i/T_i)dE_i$$

where $W_i=E_i-k_iV_i$ and $T_i=1/2\langle W_i\rangle$. The Monte Carlo selection of E_i is realized by setting

$$E_i=2T_ix+k_iV_i$$

where x is selected from the distribution x exp(-x), which is equivalent to setting x equal to one-half the sum of two random numbers on the interval (0,1). The expression for T_i, is, for neutrons,

$$T_i=1/2\left[I_2(S)+\beta I_1(S)\right]/\left[I_1(S)+\beta I_0(S)\right] \qquad (A.6.1)$$

and for charged particles,

$$T_i=1/2\cdot I_2(S)/I_1(S), \text{ where} \qquad (A.6.2)$$

$$I_2(S)=(32a^3)^{-1}(8S^3-48S^2+120S-120+e^{-S}\left[S^4-12S^2+120\right]) \qquad (A.6.3)$$

After a particle is evaporated, the procedure is repeated with updated nucleus parameters:

$$A'=A-A_i$$

$$Z'=Z-Z_i$$

$$U'=U-Q_i-E_i$$

A.3 Description of Evaporation Model Input Data

The HETC code requires an input data tape in which the first part consists of data used by the intra-nuclear-cascade model, and the second consists of data used in the evaporation model calculation. The input data arrays for the evaporation model are listed in TABLE A.4 (in the order in which they appear on the data tape), and are discussed below.

TABLE A.4

Definition of Input Data for HETC Evaporation Model

	Array	Dimension	Definition
1	P0	1001	pre-computed functions
2	P1	1001	used in evaluating
3	P2	1001	I_0, I_1, and I_2 (see text)
4	IA	6	mass numbers of possible evaporation particles
5	IZ	6	charge numbers of possible evaporation particles
6	RHO	6	radius of evaporation particles
7	OMEGA	6	(not used)
8	EXMASS	6	mass exces values (in MeV) of evaporation particles
9	CAM2	130	shell-plus-pairing energies for nuclei having charge numbers 1 through 130
10	CAM3	200	shell-plus-pairing energies for nuclei having neutron numbers 1 through 200
11	CAM4	130	pairing energies for nuclei having charge numbers 1 through 130
12	CAM5	200	pairing energies for nuclei having neutron numbers 1 through 200
13	T	3,7	constants for computing inverse cross sections (see text)
14	RMASS	297	RMASS = $A^{1/3}$, for A = 1 through 295
15	ALPH	297	ALPH = $0.76 + 1.93\ A^{-1/3}$ for A = 1 through 295
16	BET	297	BET = $(1.66A^{-2/3} - 0.05)$/ ALPH, for A = 1 through 295
17	WAPS	250,20	atomic mass data in terms of mass excess values (in MeV); WAPS(I,J) corresponds to a nuclide with mass number I=A, J = isobar index (see text)

The arrays P0, P1 and P2 are pre-computed functions which are used in evaluating the S dependence of the functions I_p, I_1, and I_2 (Eqs. (A.5.4), (A.5.5), and (A.6.3)), and are defined as follows:

$$P0=1/2\cdot\left[(S-1)\exp(S)+1\right]\exp(-50)$$

$$P1=1/8\cdot\left[(2S^2-6S+6)\exp(S)+S^2-6\right]\exp(-50)$$

$$P2=(4/32)\left[8S^3-48S^2+120S-120+\exp(-S)\cdot\right.$$
$$\left.\cdot(S^4-12S^2+120)\right]/\left[2S^2-6S+6+(S^2-1)\exp(-S)\right]$$

The values stored on tape have been computed for S=0.0 through S=100.0 in steps of 0.1, for a total of 1001 values for each array. Over this S range, the expressions in the brackets for P0 and P1 can vary over many orders of magnitude; hence, an arbitrary normalization factor of exp(-50) is included.

For all variables dependent on the evaporation particles (Items 4 through 8 in Table A.4) the order assumed is neutrons, protons, deuterons, tritons, helium-3, and alpha particles. Thus, IA=1, 1, 2, 3, 3, 4, and IZ=0, 1, 1, 1, 2, 2.

The RH0 array contains values for the radii of evaporated particles (corresponding to R_i of Eq. (A.4)) in units of 1.7 fermions. Thus, RH0(J)=0.0 for J=1 or 2, and RH0(J)=0.70588 for J=3 through 6.

The EXMASS array contains mass excess values in MeV units) for the evaporated particles, which are used in computing the Q vales of Eq. (A.5.3) in the following way. Let M(Z,A) denote he mass of an excited nucleus which evaporates a particle of mass m, leaving a residual nucleus of mass M'(Z',A'), so

$$Q=M'(Z',A')+m-M(Z,A)$$

In terms of mass excess, M(Z,A) A+ΔM(Z,A), etc., where ΔM denotes the mass excess. Therefore, Q can be written as

$$Q=\Delta M'(Z',A')-\Delta M(Z,A)+\Delta m$$

where Δm=EXMASS is the mass excess of the emitted particles. The numerical values stored are from the binding energies given in the 1964 Mass Tables /A.14/, converted to mass excess values as described in Ref. /A.7/.

The CAM arrays contain shell and pairing energy corrections, which are terms in the semi-empirical atomic mass formula of Cameron /A.13/. This formula is used to compute the mass excess of all nuclei for which data are not available from mass tables (as discussed later in connection with the WAPS array). The formula used is that given in Eq. (A.1) of Cameron's 1957 paper /A.13/:

$$\Delta M(A,Z) = [8.367A - 0.783Z + E_V + E_S + E_C + E_X] + S(Z,N) + P(Z,N)$$

Expressions for the terms E_V (volume energy), E_S (surface energy), E_C (Coulomb energy), and E_X (Coulomb exchange energy), which are functions of only Z and A, are given in Cameron's paper. In HETC, the quantity above in brackets corresponds to FUNCTION CAM(A,Z). The terms S and P are empirically determined corrections to the reference mass formula to take into account shell effects and "pairing" energies (i.e., the extra stability of nuclei with "paired" neutrons and protons). It is assumed that S and P can be written as independent functions of the neutron (N=A-Z) and proton numbers:

$$S(Z,N) = S(Z) + S(N)$$

$$P(Z,N) = P(Z) + P(N)$$

The input data arrays correspond to:

$$CAM2 = S(Z) + P(Z)$$

$$CAM3 = S(N) + P(N)$$

$$CAM4 = P(Z)$$

$$CAM5 = P(N)$$

In the code, these arrays are used in the mass formula,

$$\Delta M(Z,A)=\text{ENERGY}(A,Z) \quad \text{(code variable name)}$$

$$=\text{CAM}(A,Z)+\text{CAM2}(Z)+\text{CAM3}(A-Z)$$

and for the pairing energies alone (e.g., Eq. (A.5.3),

$$\delta=P(Z)+P(N)$$

or in the code variable names,

$$\text{CORR}=\text{CAM4}(Z)+\text{CAM5}(A-Z)$$

The numerical input values for CAM2(Z) and CAM3(N) for Z=13 through 130 and N=13 through 200 are those given in Table 1 of Cameron's 1957 paper. For Z=1 through 12 and N=1 through 12, the values given in Table 2 of Peele and Aebersold /A.15/ are used. For CAM4(Z) and CAM5(N), the values for Z=13 through 130 and N=13 through 200 correspond to (the negative of) the values in Table 1 of Cameron's 1958 paper, and the values for lower Z and N are (the negative of) the values given in Table 4 of Peele and Aebersold.

The T array contains values for the parameters used in computing inverse cross sections. The numerical values in this array are the same as given previously in TABLE A.3, with $T(1,J)=k_p$, $T(2,J)=k_\alpha$, and $T(3,J)=C_p$. The index J=1, 7 denotes the values evaluated at the seven charge number intervals given in TABLE A.3.

The next three arrays contain values for A-dependent functions evaluated at A=1 through 295. RMASS is used in computing the target nucleus radius, Eq. (A.3.4), and ALPH and BET correspond to α and β as defined in Eqs. (A.3.2) and (A.3.3). It should be noted that while these arrays are dimensioned 297, the values on tape for array locations 296 and 297 are not meaningful.

The WAPS array contains atomic mass data in terms of mass excess values in MeV units. WAPS(I,J) correspond to a nuclide with mass number I=A and J is an isobar index, which is defined as

$$J=A-2Z-J'+10, \text{ with}$$

$$J'=(A-1)/(1+124/A^{2/3})$$

where J and J' are integers.

For the data tape used with the EVAP-4 version of the evaporation model, the atomic mass data on tape are taken from the 1964 Atomic Mass Table /A.14/. For locations in the WAPS array where values are not available from the 1964 tables, they have been generated and stored in the WAPS array using the Cameron formula /A.13/. It should be noted that while the WAPS array is dimensioned 20 for each A, the J and J' algorithms for storage and retrieval are such that only 10 values are meaningful for each A. Values needed for A and Z outside of this range are computed by the code using the Cameron formula.

A.4 References

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/A.3/ I. Dostrovsky, P. Rabinowitz, and R. Bivins, "Monte Carlo Calculations of High-Energy Nuclear Interactions. I. Systematics of Nuclear Evaporation", Phys. Rev. 111, 1659 (1958).

/A.4/ I. Dostrovsky, Z. Fraenkel, and G. Friedlander, "Monte Carlo Calculations of Nuclear Evaporation Processes. III. Applications to Low-Energy Reactions", Phys. Rev. 116 683 (1959)

/A.5/ I. Dostrovsky, Z. Fraenkel, and L. Winsbert, "Monte Carlo Calculations of Nuclear Evaporation Processes. IV. Spectra of Neutrons and Charged Particles from Nuclear Reactions", Phys. Rev. 118, 781 (1960)

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/A.7/ M.P. Guthrie, "EVAP-2 and EVAP-3: Modifications of a Code to Calculate Particle Evaporation from Excited Compound Nuclei", ORNL-4379, March 1969

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/A.9/ W.E. Kinney, "The Nucleon Transport Code, NTC", ORNL-3160 (1964).

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/A.15/ R.W. Peele and P.M. Aebersold, "Energy Parameters for Light Nuclides in Monte Carlo Nuclear Evaporation Programs Based on EVAP", ORNL-TM-1538, October 1966

/A.16/ A.H. Wapstra and N.B. Gove, "The 1971 Atomic Mass Evaluation", Nucl. Data Tables 9, 265 (1971)

APPENDIX B

Input Description Cascade Model

B.1 Introduction

There are three basic types of input data required by the HETC radiation transport code: (a) target geometry and material descriptions, (b) the specification of various problem dependent transport options, and (c) a magnetic tape of problem independent data needed for the intranuclear cascade and evaporation model calculations. The purpose here is to describe the input data used by the intranuclear cascade model. This is done in anticipation of eventually updating these input data, and because the data have not been previously documented to the extent needed for making modifications. (The sources of the data used are not discussed here; they have been given by Bertini /B.1/.)

The nuclear data input tape contains 5 records of information used by the intranuclear cascade model, followed by 13 records of data pertaining to the evaporation model (Table B.1). In this chapter, we define these first 5 records; the evaporation model data arrays are defined in APPENDIX A.

In Section B.2 the input data arrays are defined, and some of the data are displayed graphically in Section B.3.

B.2 Definition of Input Arrays

A brief description of each input data array is given in Table B.2 and some further comments are given below.

Table B1

Nuclear model data arrays used as input to the HETC code. Records 1 - 5 are for the intranuclear cascade model, Records 6 - 18 for the evaporation model

Record No.	No. Words	Arrays
1	600	CRSC(1)...CRSC(600)
2	600	CRSC(601)...CRSC(1200)
3	600	CRSC(1201)...CRSC(1800)
4	600	CRSC(1801)...CRSC(2400)
5	29849	DCLN(80), DCIN(115), PPAC(19), POAC(19), FMXSN(161), FMXDN(130) FMXSP(117), PDCI(60), PDCH(55), DCHN(143), DCHNA(36), DCHNB(60), PSPCL(158), PDPCL(130), SPCLN(158), DPCLN(130), FSLN(176), FRINN(161), DMIN(101), PPSCL(117), PNSCL(117), PMSCL(117), PNNSL(117), PCFSL (234), FRIPN(117), PNMI(101), PNFSL(234), PNEC(126), PNNEC(126), PMXC(126), PMEC(126), PPEC(126), PEC(176), ECN(176), PPDC(6426), PMDD(6426), PMDX(6426), PNDD(6426)
6	3003	PO(1), P1(1), P2(1)...PO(1001), P1(1001), P2(1001)
7	12	IA(1)...IA(6), IZ(1)...IZ(6)
8	12	RHO(1)...RHO(6), OMEGA(1)...OMEGA(6)
9	6	EXMASS(1)...EXMASS(6)
10	130	CAM2(1)...CAM2(130)
11	200	CAM3(1)...CAM3(200)
12	130	CAM4(1)...CAM4(130)
13	200	CAM5(1)...CAM5(200)
14	21	((T(I,J),J=1,7), I=1,3)
15	297	RMASS(1)...RMASS(297)
16	297	ALPH(1)...ALPH(297)
17	297	BET(1)...BET(297)
18	5000	((WAPS(I,J),I=1, 250), J=1,20)

Table B2

Definition of input data arrays for the intranuclear cascade model

Array No.	Array Name	No Words	Description	Energy Range (MeV)	ΔE(MeV) for Tabulation
1.	CRSC	600	CRSC (1) through CRSC (600) contains the following nuclear data for A = 1 through 60: (a) mass number, A; (b) radial boundaries (3) defining nuclear regions, (c) nucleon density per nucleon for each region, and (d) Fermi energy per nucleon for each region.	---	---
2.	CRSC	600	CRSC (601) through CRSC (1200) contains nuclear data like Record 1 for A = 61 through 120.	---	---
3.	CRSC	600	CRSC (1201) through CRSC (1800) contains nuclear data like Record 1 for A = 121 through 180.	---	---
4.	CRSC	600	CRSC (1801) through CRSC (2400) contains nuclear data like Record 1 for A = 181 through 239. (Data included for A = 240 to fill record, but not meaningful.)	---	---
5.	DCLN	80	neutron-proton differential cross section (energy dependence of coefficients for angular distributions)	0 - 300	20
6.	DCIN	115	same meaning as Record 5	300 - 740	20
7.	PPAC	19	π^+ - p absorption cross sections (in cm^2)	0 - 360	20

Table B2 (continued)

Array No.	Array Name	No. Words	Description	Energy Range (MeV)	ΔE(MeV) for Tabulation
8.	POAC	19	π^0 - p absorption cross section (in cm^2)	0 - 360	20
9.	FMXSN	161	maximum value of pion mass distribution vs. relative kinetic energies for nucleon-nucleon single production reactions	300 - 2500	20
10.	FMXDN	130	pion mass sampling distribution for nucleon-nucleon double pion production	920 - 3500	20
11.	FMXSP	117	like record 9 but for pion-nucleon single pion production	180 - 2500	20
12.	PDCI	60	proton-proton differential cross sections, tabulated at 440, 590, 650, 800, and 1000 MeV	440 - 1000	--
13.	PDCII	55	proton-proton differential cross sections, tabulated at 1000, 1400, 2170, 2900, and 4400 MeV	1000 - 4400	--
14.	DCIBN	143	per cent scattering in backward direction for neutron-proton differential cross sections	660 - 3500	20
15.	DCINA	36	neutron-proton differential cross sections in forward direction tabulated at 630, 1540, 2560, and 3520 MeV	630 - 3520	--

Table B2 (continued)

Array No.	Array Name	No. Words	Description	Energy Range (MeV)	ΔE(MeV) for Tabulation
16.	DCHNB	60	neutron-proton differential cross sections in backward directions, tabulated at 630, 2040, 2200, 2850, and 3500 MeV	630 - 3500	--
17.	PSPCL	158	proton-proton single pion production cross sections (in cm^2)	360 - 3500	20
18	PDPCL	130	proton-proton double pion production cross sections (in cm^2)	920 - 3500	20
19.	SPCLN	158	neutron-proton single pion production cross sections (in cm^2)	360 - 3500	20
20.	DPCLN	130	neutron-proton double pion production cross sections (in cm^2)	920 - 3500	20
21.	FSLN	176	probability of producing two isobars in nucleon-proton double pion production	0 - 3500	20
22.	FRINN	161	tabulated values of integrals for isobar sampling as a function of nucleon-nucleon relative kinetic energies	300 - 3500	20
23.	DMIN	101	tabulated values of integrals for isobar sampling for nucleon-nucleon collisions as a function of the variable R, for R values from 0.0 to 1.0 in steps of 0.01	--	--

Table B2 (continued)

Array No.	Array Name	No. Words	Description	Energy Range (MeV)	ΔE(MeV) for Tabulation
24.	PPSCL	117	π^+ - proton single pion production cross sections (in cm^2)	180 - 2500	20
25.	PNSCL	117	π^0 - proton single pion production cross sections (in cm^2)	180 - 2500	20
26.	PMSCL	117	π^- - proton single pion production cross sections (in cm^2)	180 - 2500	20
27.	PNNSL	117	π^0 - neutron single pion production cross section (in cm^2)	180 - 2500	20
28.	PCFSL	234	final states for π^+ - proton single production	180 - 2500	20
29.	FRIPN	117	like Record 22 but for pion-nucleon collisions	180 - 2500	20
30.	PNMI	101	like Record 23 but for pion-nucleon collisions	--	--
31.	PNFSL	234	final states for π^0 - proton single pion production	180 - 2500	20
32.	PNEC	126	π^0 - proton elastic scattering cross sections (in cm^2)	0 - 2500	20
33.	PNNEC	126	π^0 - neutron elastic scattering cross sections (in cm^2)	0 - 2500	20

Table B2 (continued)

Array No.	Array Name	No. Words	Description	Energy Range (MeV)	ΔE(MeV) for Tabulation
34.	PMXC	126	π^- - proton charge exchange cross sections (in cm^2)	0 - 2500	20
35.	PMEC	126	π^- - proton elastic scattering cross sections (in cm^2)	0 - 2500	20
36.	PPEC	126	π^+ - proton elastic scattering cross sections (in cm^2)	0 - 2500	20
37.	PEC	176	proton-proton elastic scattering cross sections (in cm^2)	0 - 3500	20
38.	ECN	176	neutron-proton elastic scattering cross sections (in cm^2)	0 - 3500	20
39.	PPDC	6426	cummulative sampling distribution in cosθ for π^+ - proton differential cross sections	0 - 2500	20
40.	PMDD	6426	cummulative sampling distribution in cosθ for π^- - proton differential scattering cross sections	0 - 2500	20
41.	PMDX	6426	cummulative sampling distribution in cosθ for π^- - proton differential charge exchange cross sections	0 - 2500	20
42.	PNDD	6426	cummulative sampling distribution in cosθ for π^0 - proton differential scattering cross sections	0 - 2500	20

B.2.1 The CRSC Array

The first array, CRSC, contains 10 values for each target mass number, A, from A=1 through 240. (Values for A=240 are not meaningful, although values are stored just to complete the record.) For each A, the following values are stores (where i= 1,2,3):

Word Designation	Description
1	A, target mass number
2 - 4	R_i, the radial boundaries of nucleus A, dividing the nucleus into 3 regions - a central sphere and two surrounding annuli (in cm)
5 - 7	ρ_i/A, nucleon densities per nucleon for each region, divided by an arbitrary normalization factor of 10^{30} (in cm^{-3})
8 - 10	E_i^f, Fermi energy per nucleon for each region (in MeV)

The radial boundaries are defined as those radii where the nucleon density has decreased to a specified value of its central value. A continuous radial dependence of nucleon densities are assumed /B.2/:

$$\rho(r)=\rho_1\left[\exp((r-c)/Z_1)+1\right]^{-1}$$

where ρ_1= normalization factor, $c=1.07\times10^{-13}A^{1/3}$ cm, and $z_1=0.545\times10^{-13}$cm. The R_i are then defined by $\rho(R_i)=\alpha_i\rho(0)$, with $\alpha_1=0.90$, $\alpha_2=0.20$, and $\alpha_3=0.01$.

The number of neutrons or protons in each region is assumed to be the same as for the nucleus as a whole, that is,

$n_i(N)$= neutron density (per 10^{30}) in region i

$= (\rho_i/A)N$, and

$n_i(Z)$= proton density (per 10^{30}) in region i

$= (\rho_i/A)Z$

In the Fermi gas model, where the nucleus is considered as a collection of free nucleons, the Fermi momentum of particles bound in volume Ω is conventionally written as (e.g., /B.3/),

$$P_f=(3\pi^2)^{1/3}\hbar(A/\Omega)^{1/3}$$

and the corresponding kinetic energy is $E^f=(p^f)^2/2M$. The input nucleon densities correspond to $\rho_i/A=1/\Omega$, and the input Fermi energies (per nucleon) correspond to

$$\hat{E}_i^f=E^f/A=(3h^3\rho_i/8\pi)/2M$$

The Fermi energies of neutrons and protons in each region then are

$$E_i^f(N)=\hat{E}_i^f(A-Z)^{2/3} \quad \text{and}$$

$$E_i^f(Z)=\hat{E}_i^f Z^{2/3}$$

B.2.2 Differential Cross-Section Data

The differential cross section data are represented in one of three formats: (a) as expressions of the form $A+B(\cos\theta)^n$ where the coefficients are input data, (b) as tabulated values corresponding to the areas under the angular distribution in $\Delta\cos\theta$ intervals, or (c) as tabulated cummulative frequency distributions in $\mu=\cos\theta$. The method used for each cross section is given in Table B.3.

For n-p scattering, forward and backward scattering are treated separately, with the per cent of scattering in the backward direction specified by the DMHN data array. For p-p scattering, the angular distribution is assumed symmetric about $\mu=0$.

The pion-proton scattering and charge exchange cross sections are based on the phase shift data of /B.4/ and the formalism given by Bertini /B.5/. At each energy, values of μ defined by

$$R=\int_{-1}^{\mu} p(\mu)d\mu$$

are tabulated corresponding to R=0 to 1 in steps of 0.02.

Table B3

Methods used in representing differential scattering cross sections

Cross Sections	Energy (MeV)	Method	Array
$\frac{d\sigma}{d\Omega}$(n-p)	0-300	(a) forward scattering: $A_F + B_F (\cos\theta)^3$ (b) backward scattering: $A_B + B_B (\cos\theta)^5$	DCLN
	300-740	(a) forward scattering: $A_F + B_F (\cos\theta)^3$ (b) backward scattering: $A_B + B_B (\cos\theta)^5$	DCIN
	660-3520	tabulated values for $\Delta\mu$ intervals, $\mu \geq 0$	DCHNA
	660-3520	tabulated values for $\Delta\mu$ intervals, $\mu \leq 0$	DCHNB
$\frac{d\sigma}{d\Omega}$(p-p)	0-500	(assumed isotropic in center-of-mass)	---
	440-1000	tabulated values for $\Delta\mu$ intervals	PDCI
	1000-4400	(as above)	PDCH
$\frac{d\sigma}{d\Omega}(\pi^+-p)$	0-2500	cummulative frequency distributions in μ, determined from phase shift analysis	PPDC
$\frac{d\sigma}{d\Omega}(\pi^--p)$	0-2500	(as above)	PMDD
$\frac{d\sigma}{d\Omega}(\pi^0-p)$	0-2500	(as above)	PNDD
$\frac{d\sigma}{d\Omega}(\pi^--p$ c.e.)	0-2500	(as above)	PMDX

B.2.3 Data for Isobar Model

For single pion production collisions produced by an incident particle having relative kinetic energy E_r, the probability of creating an excited isobar of mass m is, according to the Sternheimer-Lindenbaum model /B.6/.

$$P(m,E_r)=C\sigma_{3/2}(m)F(m,E_r)$$

where C is a normalization constant, $\sigma_{3/2}(m)$ is the total cross section for the pion-nucleon system (evaluated at the pion kinetic energy corresponding to the total system center-of-mass energy m), and F is the phase space available. The arrays FMXSN and FMXSP pertain to selecting from the F distribution for incident nucleons and pions, respectively. The arrays FRINN and DMIN are used in selecting from σ for nucleon-nucleon collisions, and FRIPN and PNMI are used in selecting from σ for pion-nuclear collisions.

For double pion production, the masses of the isobars are expressed as

$$P(m_1,m_2,E_r)=k\sigma_{3/2}(m_1)\sigma_{3/2}(m_2)F(m_1,m_2,E_r)$$

and the FMXDN array contains data needed in selecting from F.

The three remaining input arrays containing data used by the isobar pion production model are FSLN, PCFSL, and PNFSL, which are related to specifying final states. FSLN is the probability of two isobars in nucleon-nucleon collisions, PCFSL is for π^--p final states, and PNFSL is for π^0-p final states.

B.3 Plots of Input Data

Some of the input data are shown graphically in Figs. B.1 to B.9. The points shown in these graphs are the data points of the input data -- e.g., the data points vs. energy are at the energy values of the input data without any extrapolation or interpolation.

Figs. B.1 to B.3 show the contents of the CRSC input array. The total cross sections for all reactions are shown in Figs. B.4 to B.7.

The differential cross section data have not been plotted but in Figures B.8 and B.9 the angular distributions for low-energy n-p scattering are shown. These distributions are normalized to unity in both the forward and backward directions.

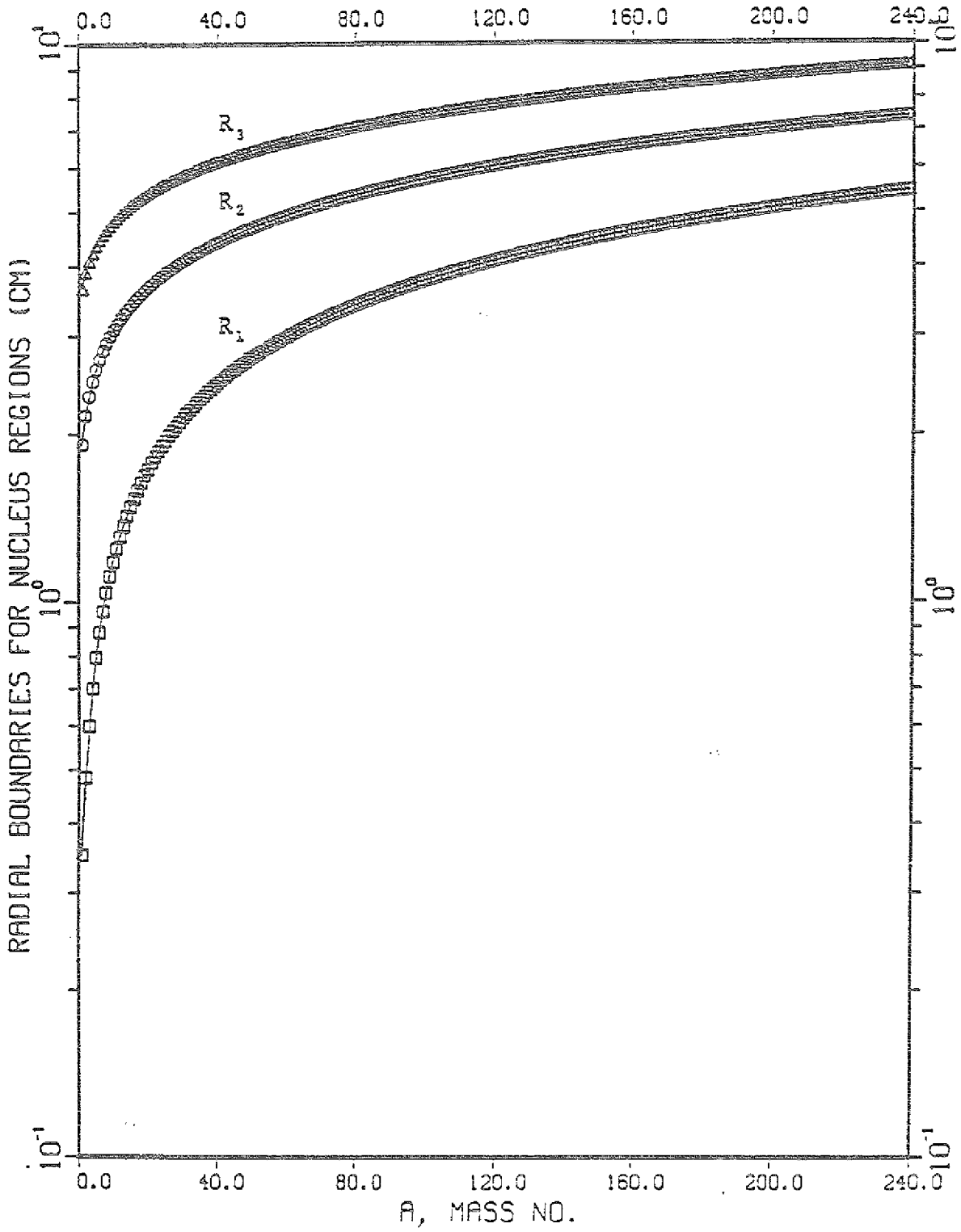

Fig. B1

Input data (CRSC array) for radial boundaries defining regions of the nucleus. (Input values have been multiplied by 10^{13} before plotting)

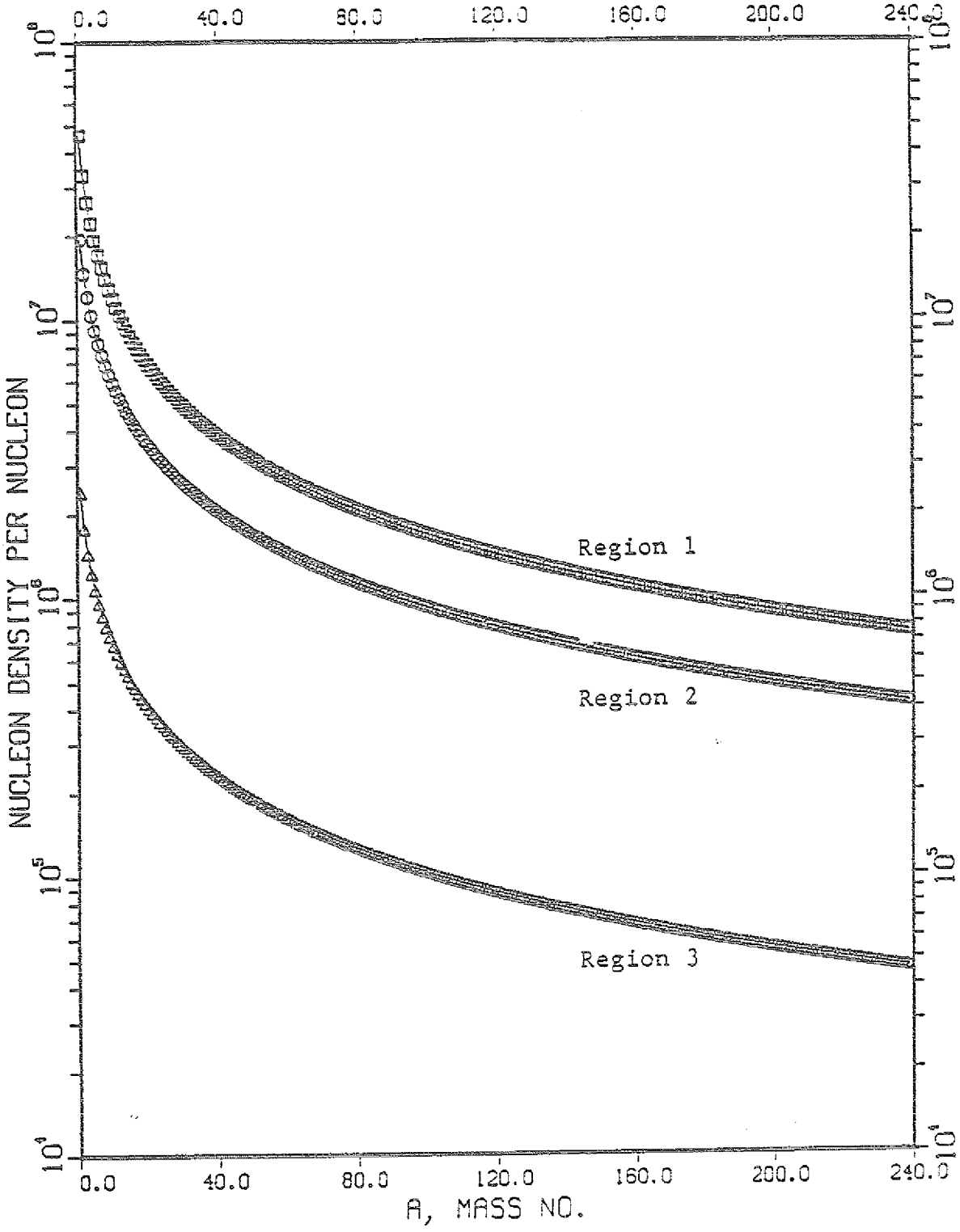

Fig. B2

Input data (CRSC array) for nucleon density in each region of the nucleus. (The input values, and the values plotted, are divided arbitrarily by 10^{30})

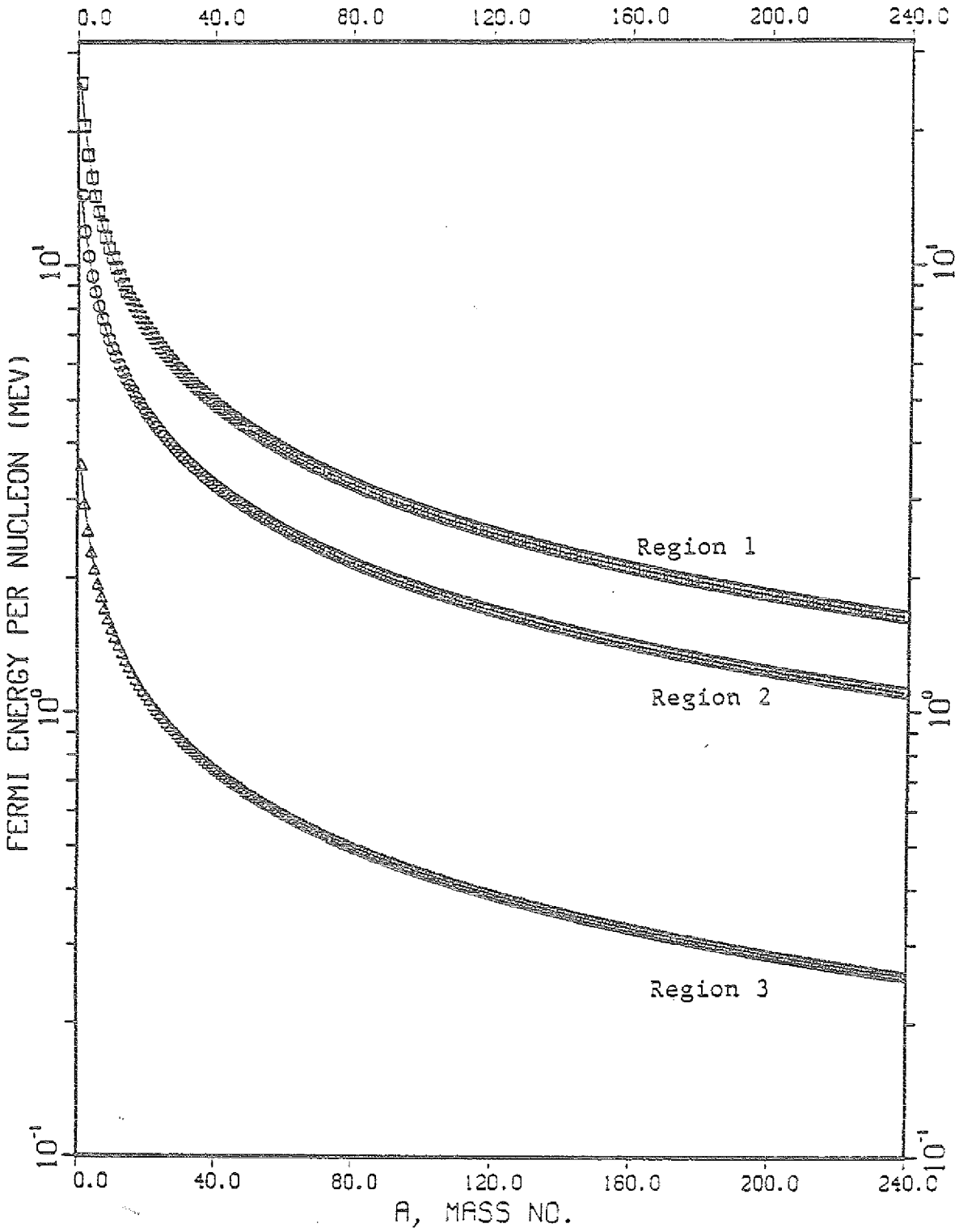

Fig. B3

Input data (CRSC array) for Fermi energy per nucleon in each region of the nucleus

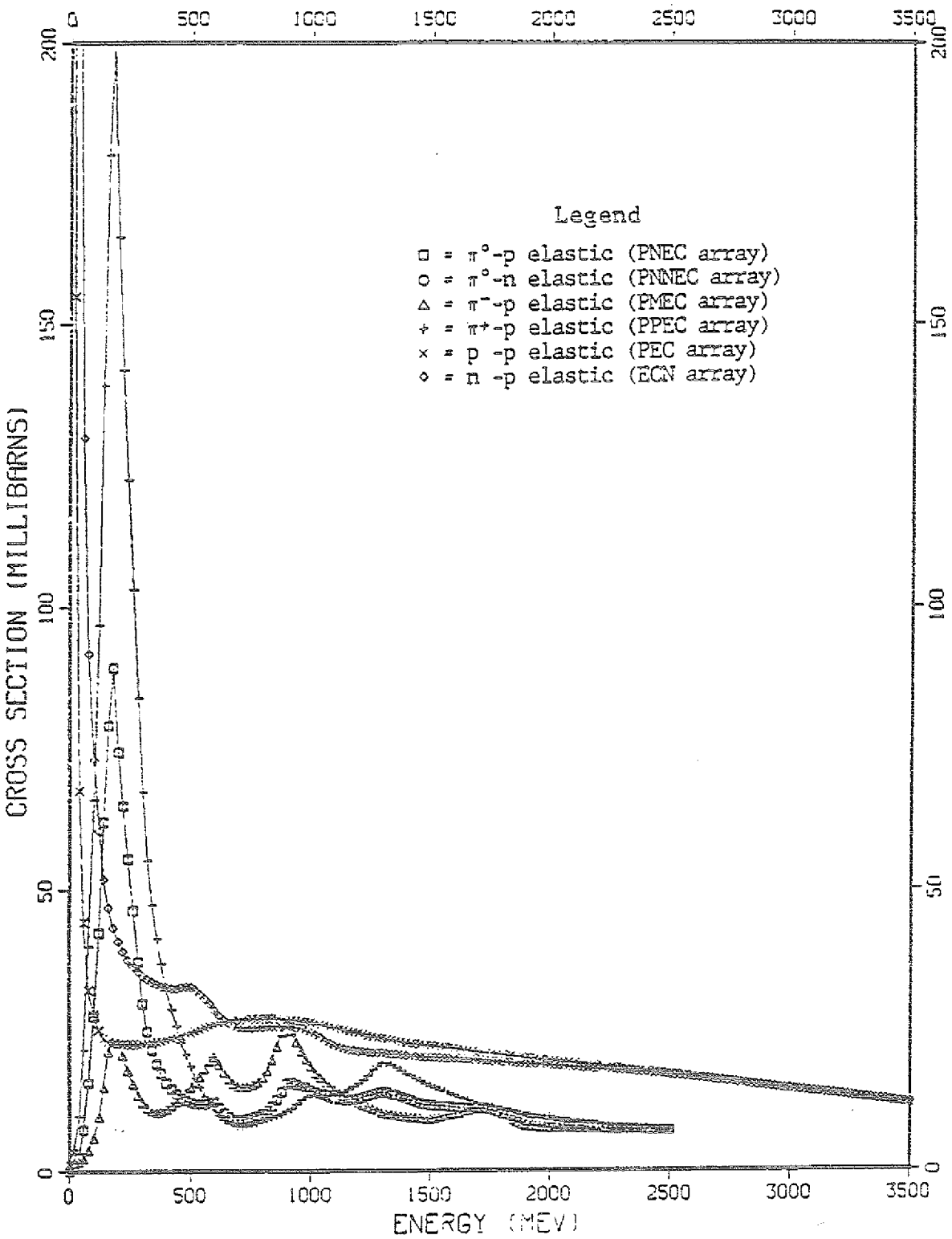

Fig. B4

Input data used for pion-nucleon and nucleon-nucleon elastic scattering cross sections. (The low-energy region is shown expanded in Figure B5)

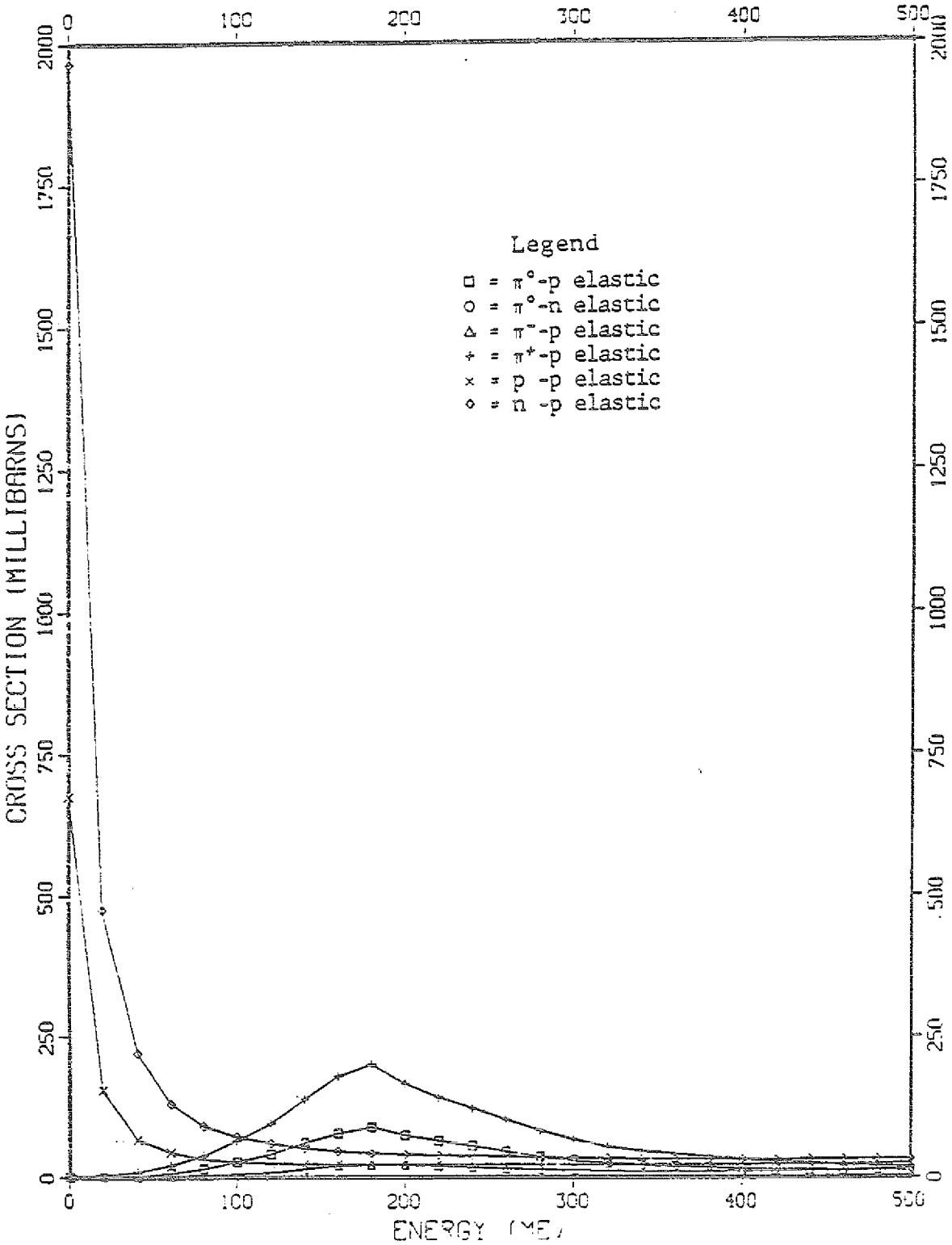

Fig. B5

Pion-nucleon and nucleon-nucleon elastic scattering cross sections in the 0 to 500 MeV energy region

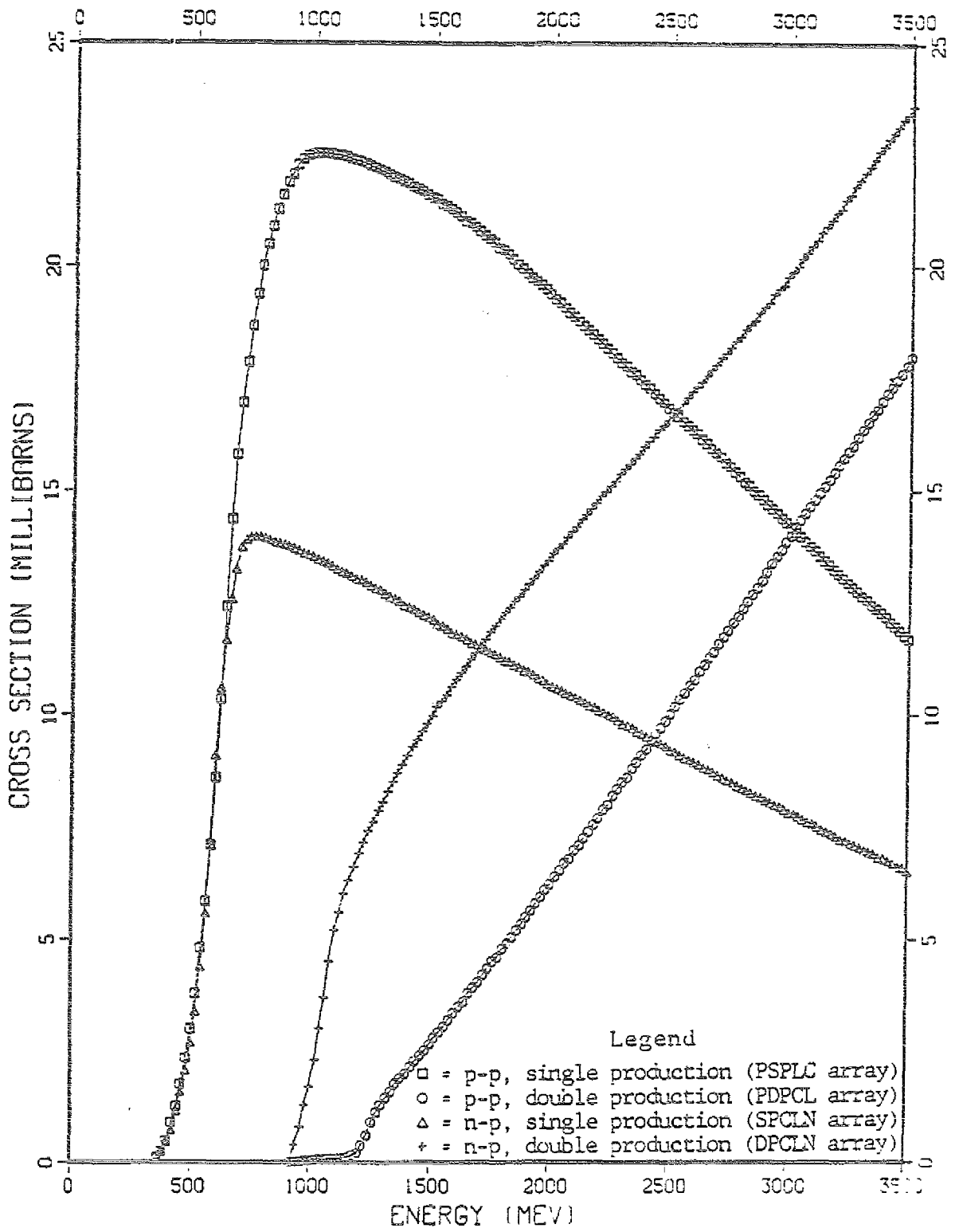

Fig. B6

Input data used for pion production cross sections for nucleon-nucleon collisions

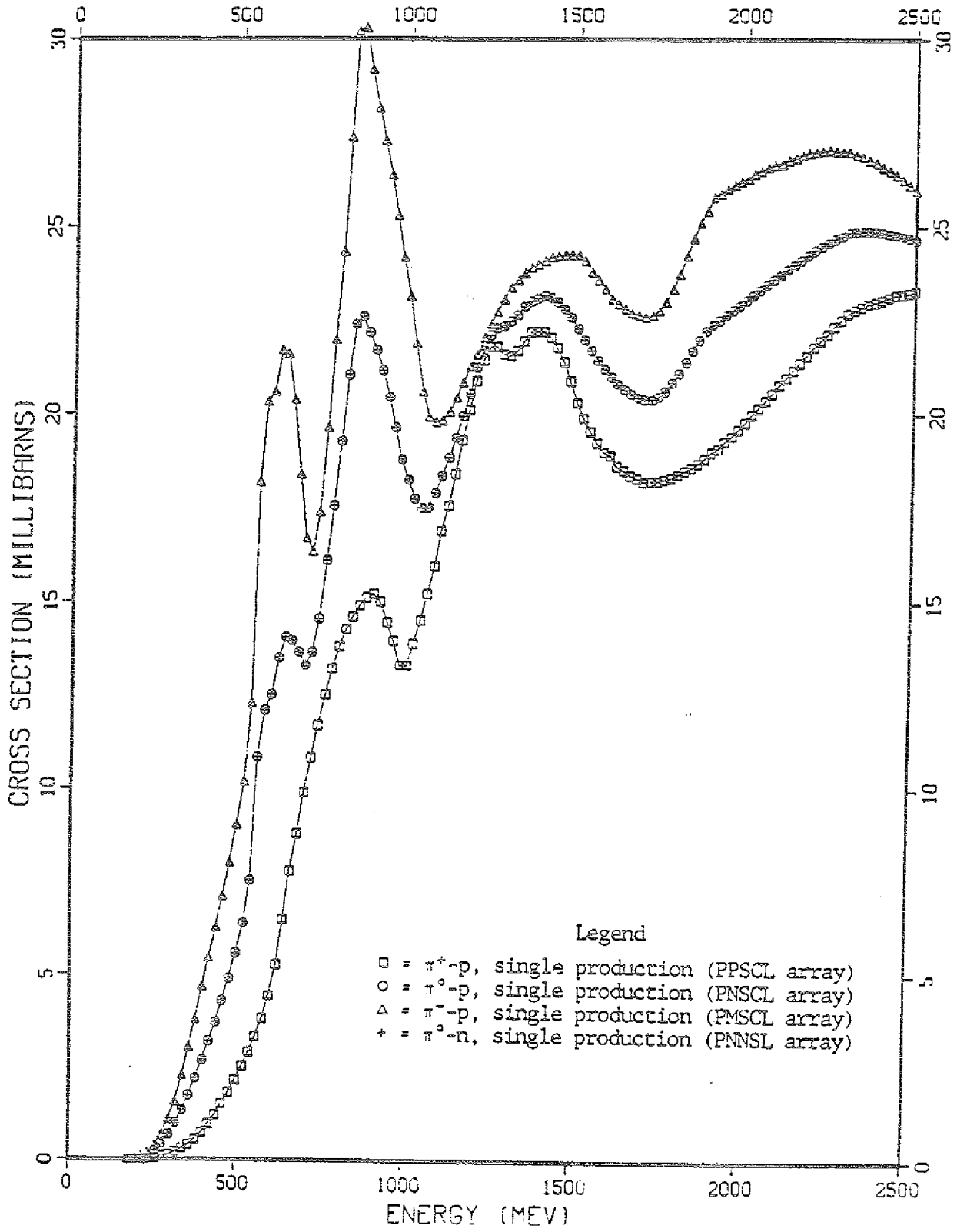

Fig. B7

Input data used for pion production cross sections for pion nucleon collisions

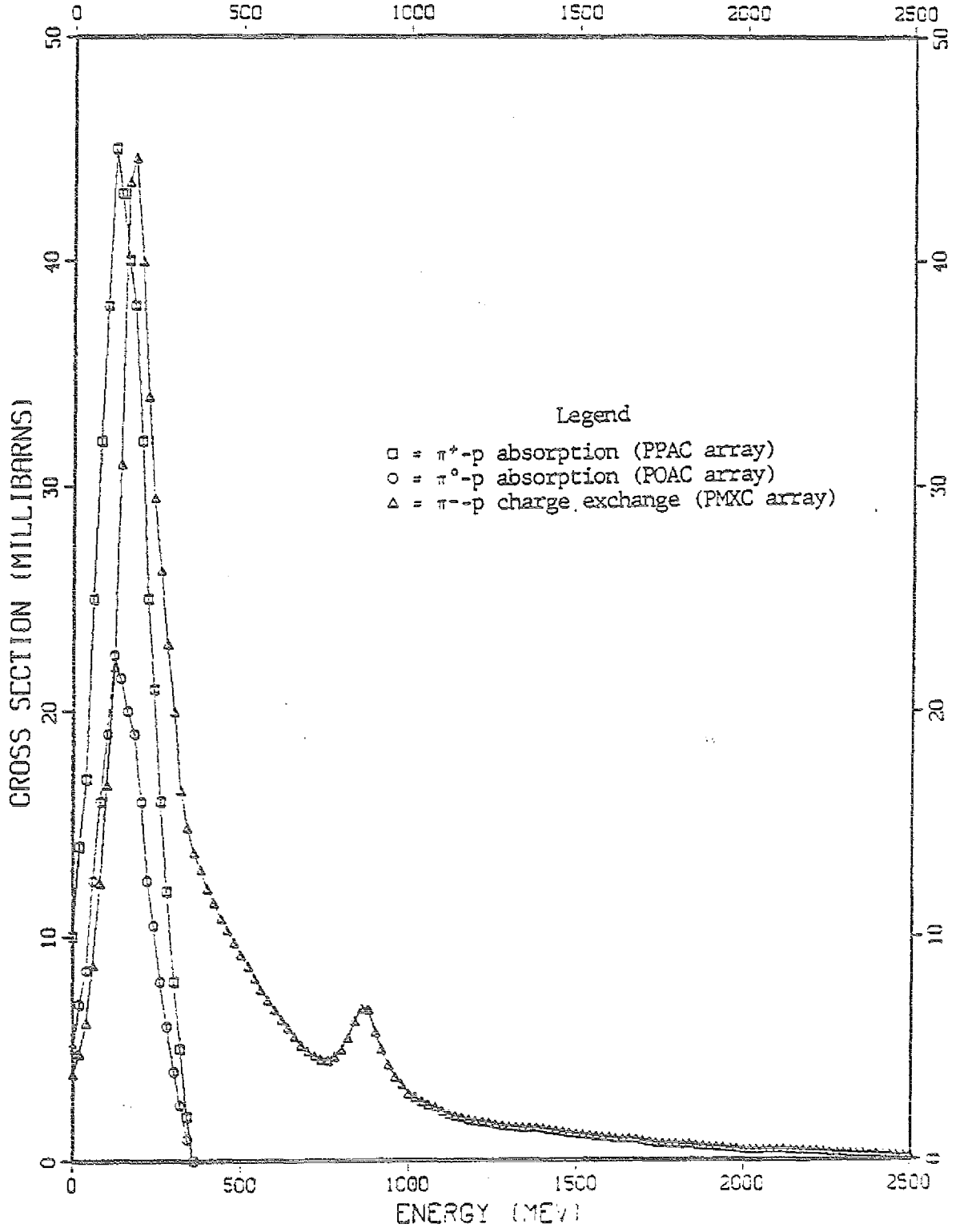

Fig. B8

Input data used for pion absorption and charge-exchange cross sections

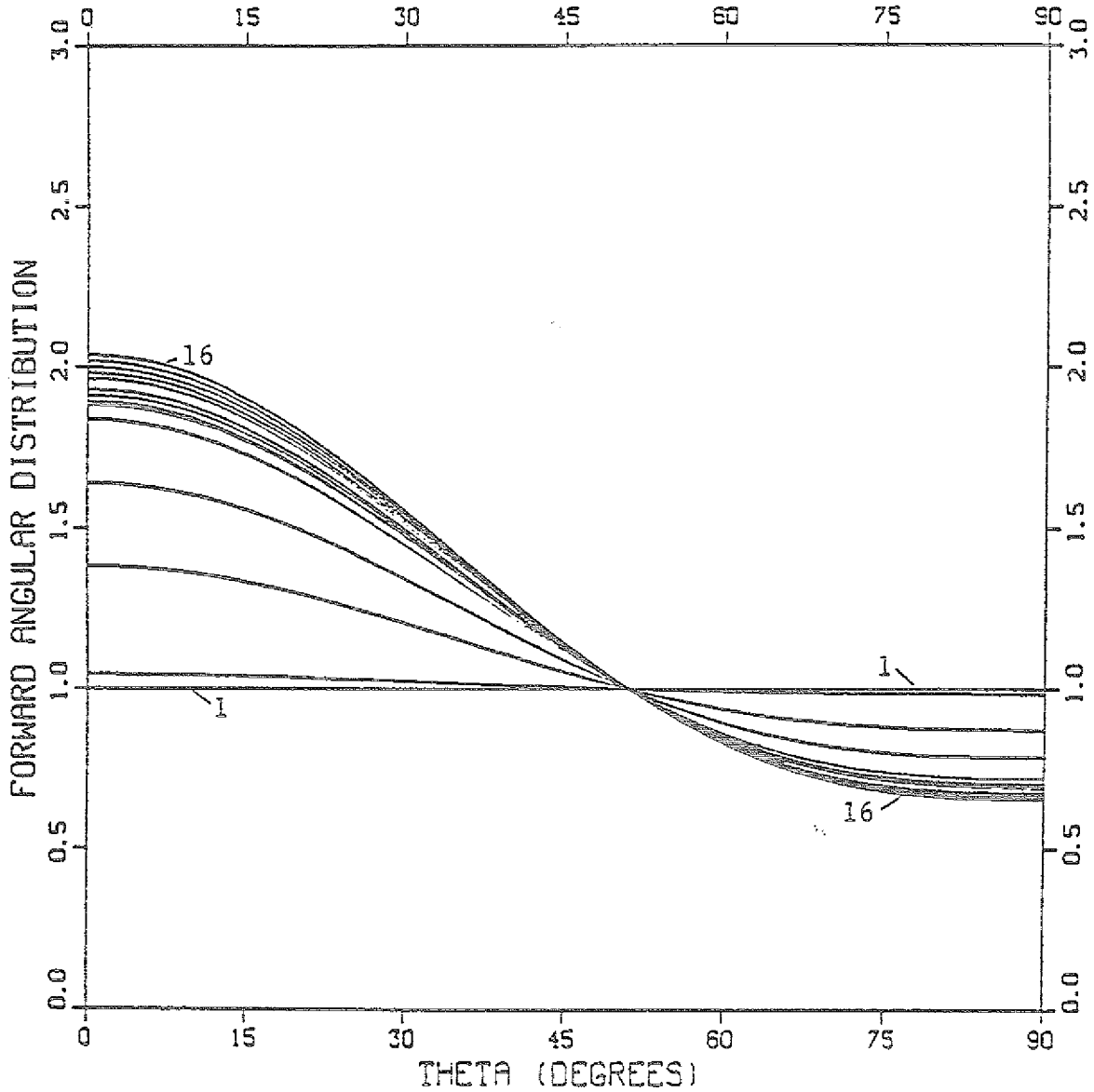

Fig. B9

Neutron-proton angular distributions (in-center-of-mass) in the forward direction for the 0 - 300 MeV range. These distributions are determined by input coefficients in the DCLN array. The curves labeled 1 and 16 are for 0 and 300 MeV, respectively, and the intermediate curves are at 20 MeV intervals.

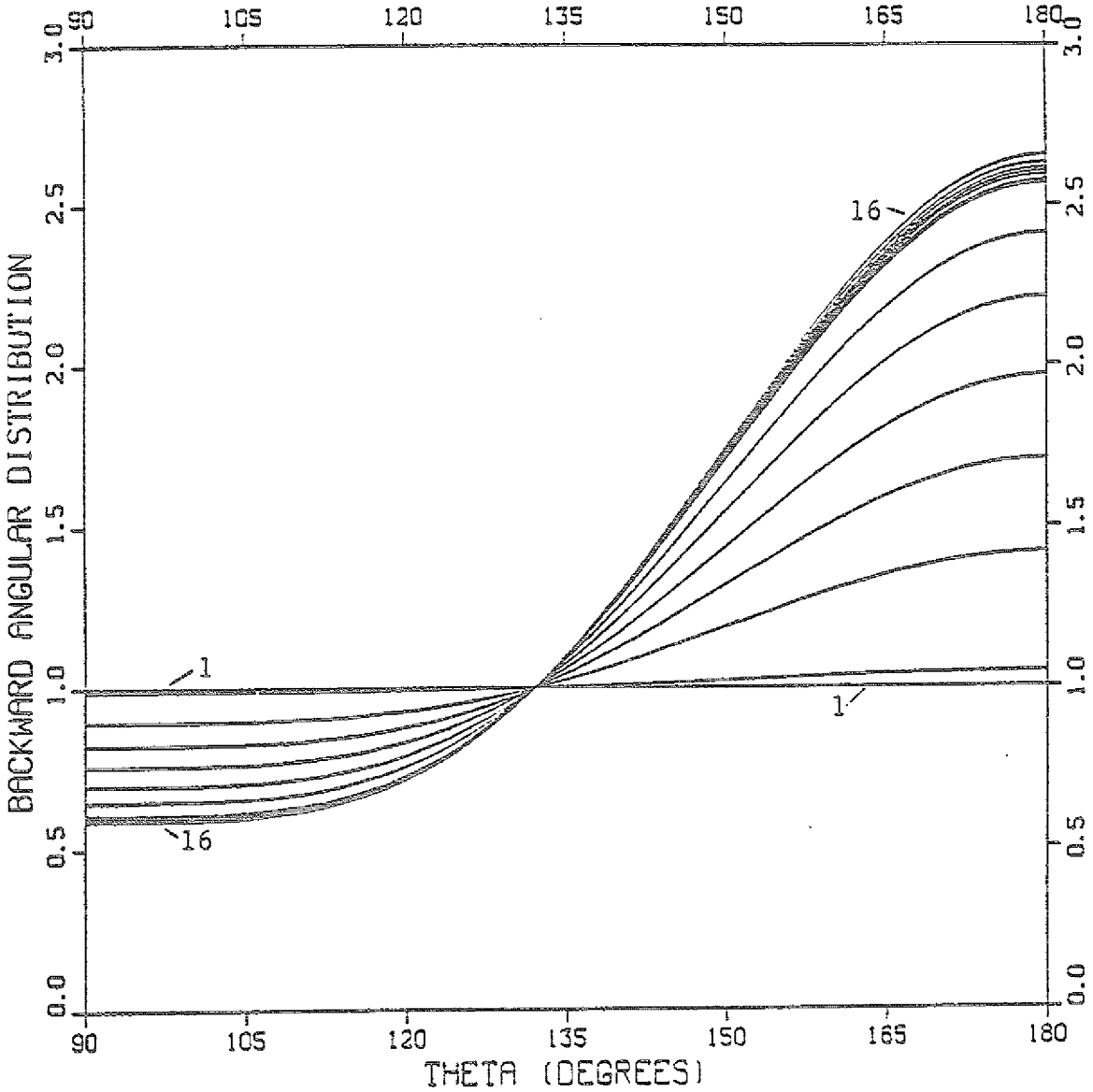

Fig. B10

Like Figure B9 but for backward directions

B.4 References

/B.1/ H.W. Bertini, "Intranuclear-Cascade Calculations of the Secondary Nucleons Spectra From Nucleon-Nucleus Interactions in the Energy Range 340 to 2900 MeV and Comparisons with Experiment", Phys. Rev. 188, 1711 (1969)

/B.2/ R. Hofstadter, 28, 214 (1956)

/B.3/ E. Segre, Nuclei and Particles, W.A. Benjamin, Inc., Reading, Mass., 1977

/B.4/ A. Donnachi, R.G. Kirsopp, and C. Lovelace, "Evidence from Pi-P Phase Shift Analysis for Nine More Possible Nucleon Resonances", CERN Report 67/1285/5-TH838, Oct. 1969

/B.5/ H.W. Bertini, "Pion-Nucleon Differential Cross Sections in the 0 to 700 MeV Energy Region in Terms of Coulomb Scattering Amplitude, Coulomb Phase Shifts, and Nuclear Phase Shifts up to l = 4", ORNL-4197, January 1968

/B.6/ R.M. Sternheimer and S.J. Lindenbaum, "Extension of the Isobaric Nucleon Model for Pion Production in Pion-Nucleon Nucleon-Nucleon, and Antinucleon-Nucleon Interactions", Phys. Rev. 123, 333 (1961)

APPENDIX C
The Combinatorial Geometry

C.1 General Design

CG-GEOM is a Program used to describe a three dimensional geometry and to control tracing of particles (or points) through this geometry.

CG-GEOM provides a set of 'bodies', which may be located and described by parameters as their spatial location and orientation and size parameters as radius etc.

The 'bodies' are combined to 'geometry zones'. Thus each zone is described by a list of bodies to be included in,or excluded from the zone.

The 'geometry zones' are assigned to 'media' and 'regions', where a 'medium' normally includes one single material, and the 'regions' are used to define special volumes of interest, for example detectors.

Normally the geometry routines are called by random-walk routines of a monte-carlo transport code or by a three dimensional analysis code (as SIMPEL), to find the appropriate 'medium' cross sections or the 'region' to activate the appropriate detector.(see also Ref. /4/)

C.2 Standard Program Interface to Use CG-GEOM

There are three subroutine calls, the named common /GEOMC/ and the blank common needed to use CG-GEOM.

- SUBROUTINE JOMIN (IADD,IN,IOUT)
  which reads the geometry data from unit IN, into the blank common starting at location IADD.
  When JOMIN returns, the blank common location IADD contains the number of storage words used.
  The call of JOMIN must preceed any other use of the geometry.
  The processed input data is reported on unit IOUT.

- SUBROUTINE LOOKZ (X,Y,Z)
  which computes the region and medium number for a starting point at (X,Y,Z), where X,Y,Z are given in double precission
  LOOKZ must be called for each particle at the beginning of its walk.
- SUBROUTINE GEOM
  which traces a particle from a given starting point (X1,Y1,Z1) along the direction (X2,Y2,Z2) - (X1,Y1,Z1) until the given tentative 'end-of-flight point' (X2,Y2,Z2) is reached or a geometry boundary is crossed. GEOM needs IBLD at the particle's position (X1,Y1,Z1).

  IBLD will be avaiable after a call of LOOKZ or must be set by the user.

- COMMON /GEOMC/ X2,Y2,Z2,X1,Y1,Z1,ETA,ETAUSD,IBLZ,IBLZD, MARC,NMED,NREG

```
REAL*8 X2,Y2,Z2,X1,Y1,Z1,ETA,ETAUSD
```

If the 'tentative end of flight point' is reached GEOM will return with

```
  MARC   = 1
ETAUSD = number of distance units ETA used for this path
  NMED   = medium number of the current geometry medium
  NREG   = region number of the current geometry region
  IBLZ   = internal code-zone number of the current zone
  IBLD   = IBLZ
```

For a subsequent call of GEOM for the same particle, IBLD is allready o.k.

If a boundary crossing is detected GEOM will return with

```
  MARC   = 0  for internal boundaries
         =-1  for boundary crossing into external void
         =-2  for boundary crossing into internal void
  ETAUSD = number of distance units ETA used for this path
  NMED   = medium number of medium to be entered
  NREG   = region number of region to be entered
  IBLZ   = internal code-zone number of current zone
  IBLD   = internal code-zone number of next zone to be
           entered
```

X2,Y2,Z2= coordinates of boundary crossing point.

For a subsequent call of GEOM for the same particle, the user has to set IBLD=IBLZ.

C.3 Extended Interface to CG-GEOM

In addition to the above interface ,the user can get information about the normal vector of the crossed surface at the crossing point in case of boundary crossing, and about zone volumes.

- SUBROUTINE NORMV
  will return the normal vector at the crossing point on common
- COMMON /NORMAL/ UN,VN,WN
  REAL*8 UN,VN,WN

NORMV must be called immediatly after the boundary crossing occured.

- SUBROUTINE GTVOL (MAX,GNOR)
  REAL*4 GNOR (MAX)
  will return the volumes of the first MAX zones on the array GNOR.

Note: In the current version of CG-GEOM, volumes are read in or set equal to one according to the input.
In SIMPEL the user won't use this method.
In a later release, there will be a module, which computes region or media volumes and inter-region or inter-media surfaces.

C.4 CG-GEOM Input Instructions

The input is read from unit IN as specified in the JOMIN-call, i.e. in SIMPEL this will be the unit specified in the GEOIN-command.

Card 1 :Format(7I5)

NUMB	= number of bodies
NUMR	= number of input geometry zones
NCOD	= number of code zones = NUMR + number of OR operators used

LMXX = maximum length of floating point array FPD
(the used length will be printed out)
LMYY = maximum length of integer array MA
LOUT = not used in this version

Card 2 :Format(2I6)

IVOPT = 0 --> set all volumes equal to 1.0
= 1 --> invalid in this version
= 2 --> invalid in this version
= 3 --> read in NUMR volumes
= 4 --> bypass volume determination

MEDREG =-1 --> return from GEOM at region-boundary crossing only
= 0 --> return from GEOM at all boundary crossings
= 1 --> return from GEOM at medium-boundary crossing only

Note: for HETC use IVOPT=4 and MEDREG=1
for SIMPEL use IVOPT=4 and MEDREG=0

Card 3 :Format(I10,E15.4,A3,13A4)

IPRINT = 1 --> print out geometry description
= 0 --> no print

STRETCH = all body parameters will be multiplied by this factor

TITLE = text to identify the input

Card(s) 4 :Format(2X,A3,1X,I4,6E10.3)

TYPE = body-type name

INR = body number

PRARM = parameters describing the body

Note: Card 4 is repeated for NUMB bodies.
The last one must be 'END'.
If a body requires more than six parameters, one or more continuation lines must be used leaving TYPE and INR blank.
See table BODIES to find the parameters needed for the body input

Card(s) 5 :Format(2I5,9(A2,I5))

IMED = medium number for this input zone

IREG = region number for this input zone

(IOR_i, $IBODY_i$)

Note: An input zone consists of one or more code zones. Each code zone 'CZ' describes a set of spatial points:

$(x_{CZ}, y_{CZ}, z_{CZ}) \in CZ$

A point lies within an input zone, when it lies in one of the code zones defining the input zone.
If an input zone consists of more than one code zone, each code zone description must be preceeded by OR.

A code zone is defined by one or more bodies IBODY, describing a set of spatial points

$(x_{IBODY}, y_{Ibody}, z_{IBODY}) \in IBODY$

If IBODY > 0 : all (x_{CZ}, y_{CZ}, z_{CZ}) must lie within IBODY
If IBODY < 0 : all (x_{CZ}, y_{CZ}, z_{CZ}) must lie outside IBODY

If more than one card (i.e. 9 bodies) is needed to specify an input zone, a continuation line must be used leaving IMED and IREG blank.

IMED = 1000 specifies an internal void: (vacuum)
IMED = -1 specifies external void.
IMED = 999 terminates the zone input.

Card(s) 6 :Format(7E10.5) (omitt if IVOPT'=3)

VNOR = NUMR volumes of the input zones

TABLE C.1

CG-Body Types

Body type	TYPE	PARAM					
box	BOX	v_x	v_y	v_z	h_{1x}	h_{1y}	h_{1z}
		h_{2x}	h_{2y}	h_{2z}	h_{3x}	h_{3y}	h_{3z}
right parallel-epiped	RPP	x_{min}	x_{max}	y_{min}	y_{max}	z_{min}	z_{max}
sphere	SPH	v_x	v_y	v_z	r		
right circular cylinder	RCC	v_x	v_y	v_z	h_x	h_y	h_z
		r					
right elliptic cylinder	REC	v_x	v_y	v_z	h_x	h_y	h_z
		r_{1x}	r_{1y}	r_{1z}	r_{2x}	r_{2y}	r_{2z}
ellipsoid	ELL	v_{1x}	v_{1y}	v_{1z}	v_{2x}	v_{2y}	v_{2z}
		b					
truncated right cone	TRC	v_x	v_y	v_z	h_x	h_y	h_z
		r_1	r_2				
right angle wedge	WED or RAW	v_x	v_y	v_z	h_{1x}	h_{1y}	h_{1z}
		h_{2x}	h_{2y}	h_{2z}	h_{3x}	h_{3y}	h_{3z}
arbitrary polyhedron	ARB	v_{1x}	v_{1y}	v_{1z}	v_{2x}	v_{2y}	v_{2z}
		v_{3x}	v_{3y}	v_{3z}	v_{4x}	v_{4y}	v_{4z}
		v_{5x}	v_{5y}	v_{5z}	v_{6x}	v_{6y}	v_{6z}
		v_{7x}	v_{7y}	v_{7z}	v_{8x}	v_{8y}	v_{8z}
		s_1^4	s_2^4	s_3^4	s_4^4	s_5^4	s_6^4

where

(v_x, v_y, v_z)	is a vertex vector
(h_x, h_y, h_z)	is a hight vector
r	is a scalar radius
(r_{ix}, r_{iy}, r_{iz})	is an ellipsis radius
s_i^4	is a four digit real number where each digit is the index of a vertex vector v_i of the corner of a plane area.

APPENDIX D
The PICTURE-CG Progam

PICTURE produces line-printer-plots of plane cuts through a three-dimensional geometry described by the combinatorial geometry module CG-GEOM.(see Ref. /4/)

Its purpose is the checking and presentation of the geometry.

D.1 Input for PICTURE

Input to picture is read from unit IN specified in the PICTURE command.

```
Card 1   :Format(I5)
          NNUSE     =0  use the default symbol table.
                    >0  read in a new symbol table with NNUSE
                        entries.
                        (NNUSE must be less than or equal 200)

Card(S) 2:Format(40A2) (omit if NNUSE.le.0)
          ATABLE        symbol table of length NNUSE

Card(s) 3:omit if SIMPEL is used.
          insert CG-geom input here for the stand alone vers-
          ion of PICTURE

CARD 4-1 :Format(2I2,18A4)
          IOPT      <0  stop
                    =0  continue reading the next frame speci-
                        fication (card set 4 ).
                    >0  continue reading the next geometry des-
                        cription (card set 3 ).
          IRG       =0  print out media-geometry
                    ^=0 print out region-geometry
          TITLE         text to identify the picture frame.

Card 4-2 :Format(6E10.5)
          XO            coordinates of upper left corner of the
          YO            frame
          ZO
          X1            coordinates of lower right corner of
          Y1            the frame
          Z1
```

Card 4-3 :Format(6E10.5)

XU	direction cosines of the u-axis
YU	"
ZU	"
XV	direction cosines of the v-axis
YV	
ZV	

Card 4-4 :Format(2I5,2E10.5)

NU	number of characters in U direction
NV	number of characters in V direction
DELU	spacing of U-axis
DELV	spacing of V-axis

(specify either NU,NV or DELU,DELV)

input continues according to IOPT.

D.2 Method of Operation

According to the symbol table each region or medium of the geometry is connected with a special character to be printed.

The U and V axes define a plane area through the geometry, with U=0 and V=0 in (X0,Y0,Z0). NU beams are traced along this plane.

They are started at the coordinates

$$(X_i,Y_i,Z_i) = (X0,Y0,Z0) + (i-1) * DELU * (XU,YU,ZU) \quad i=1,NU$$

LOOKZ is called to ask for the region and medium number of the starting point. According to these numbers a character C is selected from the symbol table.

The beam direction is given as (XV,YV,ZV).

The space unit for the geometry routines is set to DELV. Then GEOM is called to trace the beam to the next geometry boundary. GEOM returns the variable ETAUSD which is the number of space units (i.e. characters) used until the boundary crossing occurs. So ETAUSD characters C may be stored into the print buffer. A new character C is selected according to the region or medium number of the next zone to be entered as known from GEOM.

This procedure is repeated until the beam reaches the other side of the plane area at :

$$(X_j, Y_j, Z_j) = (X0, Y0, Z0) + (i-1) * DELU * (XU, YU, ZU) + NV * DELV * (XV, YV, ZV)$$

PICTURE may be used also for other geometry modules, if those use the same program interface as CG-GEOM;
(see APPENDIX C)

APPENDIX E

Sample Problem

E.1 Introduction

This sample problem considers a 350 MeV proton beam incident on a slab containing a mixture of depleted uranium, water and aluminum. The composition is 76.5 % U, 16.5 % H_2O and 7 % Al. The slab has dimensions of 10 x 30 x 80 cm^3. The beam axis is perpendicular to the front face of 10 x 30 cm^2 of the slab. In the following a listing of input data and output of the SIMPEL program with an edit for total yields, volume fluxes, surface currents and total energy depositions for all particles is given. The problem was run on the IBM 370/3033 computer at KFA. The job control language is that of the MVS system under JES2.

E.2 Elastic Scattering Data Input

```
//REW03100 JOB (152,011881),STERZENBACH,TIME=(,30)
/*JOBPARM  L=15
/*ROUTE  PRINT R9
//*
//*       SUBMIT.ELAS.TRG01
//*              ELASTIC N-SIGMA.SCAT FOR AL,O
//*
//ERASE  EXEC AMSCMD
//SYSIN DD *
   DEL 'USRT.REW031.ELAS.TRG01'
/*
//ALLOC  EXEC PGM=IEFBR14,COND=(9,LT)
//NEWDS  DD   UNIT=3330V,MSVGP=TMSS0404,DISP=(NEW,CATLG),
//     DCB=(RECFM=FB,LRECL=80,BLKSIZE=6160),
//     DSN=USRT.REW031.ELAS.TRG01
//WRITE1 EXEC GFORT,NAME=PUNCHWQ,DS='USER.REW30LOD',COND=(9,LT)
//G.FT10F001 DD DSN=USER.REW031.O5RDAT(O5RHET),DISP=SHR
//G.FT11F001 DD DSN=USRT.REW031.ELAS.TRG01,DISP=SHR
//G.SYSIN    DD *
   10   11    1
      14.9      100.
13000    2       AL-NAT ELASTIC
13000   71              F1
 8000    2        O- 16 ELASTIC
 8000   71              F1
    0    0       END OF DATA
/*
```

E.3 HETC/KFA-1 Input

```
//REW031T2 JOB (152,011881),STERZENBACH,TIME=(64),REGION=2000K
/*JOBPARM  L=15
/*ROUTE  PRINT R9
//*------->SUBMIT.HETN.TRG01B   EO=350MEV SNQ 2-DESIGN
//*****************************************************************
//*------->ERASE OLD MSS-DATASETS
//      EXEC AMSCMD
//SYSIN DD *
   DEL 'USRT.REW031.HTRG01B'
   DEL 'USRT.REW031.NTRG01B'
/*
//*------->ALLOCATE NEW MSS-DATASETS
//      EXEC PGM=IEFBR14,COND=(9,LT)
//NHSTP DD  DSN=USRT.REW031.HTRG01B,DISP=(NEW,CATLG),
//       UNIT=3330V,MSVGP=TMSS8008,DCB=(RECFM=VBS,BLKSIZE=3020)
//NEUTP DD  DSN=USRT.REW031.NTRG01B,DISP=(NEW,CATLG),
//       UNIT=3330V,MSVGP=TMSS0404,DCB=(RECFM=VBS,BLKSIZE=3020)
//*------->RUN HETN
//*      HERE AN CG-LIKE SPECICAL GEOMETRY IS USED TO SPEED UP
//*      THE CODE
//HETN EXEC CLGFORTE,COND=(9,LT),PARM.C='XREF,MAP,OPTIMIZE(2)'

      SUBROUTINE LOOKZ (X,Y,Z)
C-----------------------------------------------------------------------
C     MODULE =SLAB1    (SINGLE SLAB)
C     SUBNAME=LOOKZ
C-----------------------------------------------------------------------
      REAL*8             X,Y,Z
      COMMON    /GEOMC/ X2(3),X1(3),ETA,ETAUSD,IBLN,IBLO,MARC,
     +                  NMED,NREG
      REAL*8             X2,X1,ETA,ETAUSD
      COMMON    /SLB1/  XMIN,YMIN,ZMIN,XMAX,YMAX,ZMAX,XLEN,YLEN,ZLEN,IO
C-----------------------------------------------------------------------
      MARC  =1
      IF    (X.LT.XMIN .OR. Y.LT.YMIN .OR. Z.LT.ZMIN) GOTO 1
      IF    (X.GT.XMAX .OR. Y.GT.YMAX .OR. Z.GT.ZMAX) GOTO 1
      NMED  =1
      NREG  =1
      RETURN
    1 CONTINUE
      WRITE (IO,600) X,Y,Z
  600 FORMAT('--GEO--> LOOKZ : CALLED WITH INVALID POINT'/
     +       '                 ',1P3D10.3)
      MARC  =-1
      NMED  =0
      NREG  =0
      RETURN
      END
```

```
      SUBROUTINE GEOM
C-----------------------------------------------------------------------
C     MODULE =SLAB1
C     SUBNAME=GEOM
C     SUBNAME=NORMV
C-----------------------------------------------------------------------
      COMMON    /GEOMC/ X2(3),X1(3),ETA,ETAUSD,IBLN,IBLO,MARC,
     +                  NMED,NREG
      REAL*8            X2,X1,ETA,ETAUSD
      COMMON    /SLB1/  XYZLIM(3,2)                    ,XLEN,YLEN,ZLEN,IO
      COMMON    /NORMAL/UN(3)
      REAL*8            UN
      REAL*8            ROOT,PTH,USE,U(3)
C-----------------------------------------------------------------------
      MARC=1
      USE   =0.DO
      DO 1 I=1,3
           U(I) = X2(I) - X1(I)
           USE  = USE   + U(I)**2
    1 CONTINUE
      USE   =DSQRT (USE)
      PTH   =USE
      DO 20 I=1,3
         U(I)  =U(I) /USE
         IF    (U(I))          11,20,13
   11          ROOT  =(XYZLIM(I,1)-X1(I)) / U(I)
               J     =-I
             GOTO  15
C  12         ROOT  = 1.E72
C            GOTO  15
   13          ROOT  =(XYZLIM(I,2)-X1(I)) / U(I)
               J     =I
   15    IF    (ROOT.GE.PTH)      GOTO 20
         PTH   =ROOT
         ISURF =J
         MARC  =-1
   20 CONTINUE
      IF    (MARC)    2,2,5
    2 NREG  =0
      NMED  =0
      ETAUSD=PTH /USE *ETA
      DO 3 I=1,3
           X2(I) = X1(I) + PTH * U(I)
    3 CONTINUE
      ENTRY NORMV
      DO 4 I=1,3
           UN(I)  = 0.
    4 CONTINUE
      UN (IABS(ISURF)) = ISURF
      RETURN
    5 CONTINUE
      NMED  =1
      NREG  =1
      ETAUSD=1.DO
      RETURN
      END
      SUBROUTINE JOMIN (IAD,IN,IO)
```

```
C-----------------------------------------------------------------------
C      MODULE =SPH1
C      SUBNAME=JOMIN
C-----------------------------------------------------------------------
       COMMON      I4C(1)
       COMMON     /SLB1/ XMIN,YMIN,ZMIN,XMAX,YMAX,ZMAX,XLEN,YLEN,ZLEN,IO
       NAMELIST   /GEO/  XMIN,YMIN,ZMIN,XMAX,YMAX,ZMAX,XLEN,YLEN,ZLEN
C-----------------------------------------------------------------------
       IO  =IO
       I4C (IAD) =1
       WRITE (IO,600)
  600  FORMAT('--GEO--> JOMIN : YOU ARE USING SLAB1-GEOMETRY ')
       READ  (IN,GEO)
       XLEN = XMAX - XMIN
       YLEN = YMAX - YMIN
       ZLEN = ZMAX - ZMIN
       WRITE (IO,GEO)
       RETURN
       END
/*

//L.SYSIN DD *
   INCLUDE USER(HETN1)
   INCLUDE USER(HETNAL)
   INCLUDE USER(HETN)
   ENTRY   MAIN
/*

//G.SYSIN DD *
SUBMIT.HETN.TRG01B
WITH REFERNCE TARGET MATERIAL
D2E69F59D9A7
 &RUN
     MAXCAS=100, MAXBCH=100, IHOUR=1,  IMINIT=02,  ISEC=00,
 C='---------------------- ENERGIES ----------------------------------',
     EMIN(1)=14.9,EMIN(2)=14.9,EPICUT=1.,   EMUCUT=1.,   ELOP=14.9,
     CTOFE=0.,     EMAX=350.,  ELAS=100.,
 C='---------------------- TAPES -------------------------------------',
     NEUTP=10,     NHSTP=30,     IGAMTP=0,    IBERTP=-20,  NELSTP=21,
 C='---------------------- OPTIONS -----------------------------------',
     N1COL=0,      NPIDK=0,      NBOGUS=1,     NSPRED=0,     NWSPRD=0,
     NSEUDO=1,     ISTRAG=0,     IANG=0,       IFISS=1,      IB0=1,
     IGEOM=0,      NLEDIT=1,                   B0=10.,
 C='---------------------- MATERIALS ---FOR TRG01B--------------------',
     MXMAT=1, NOELAS=2,
     DENH(1)=11.1088-3,  NEL(1)=4,  NOEL(1)=2,
             ZZ=      13.,       8.,      92.,      92.,
              A=      27.,      16.,     235.,     238.,
            DEN=4.0956-3,5.5544-3,7.3663-5,3.6758-2,
             ID=         1,        2,        0,        0,
 C='----------PROTON BEAM SOURCE 350MEV F.H.W.=4CM-----------------',
  TIPSR=0.0,    XSR=0.0,    YSR=0.0,    ZSR=0.0,    ESR=350.,   WTSR=1.0,
              XSIG=1.699,YSIG=0.0,   ZSIG=1.699, ESIG=0.0,     RSR=5.0,
               USR=0.0,    VSR=1.0,    WSR=0.0
 &END
 &GEO XMIN=-15.,XMAX=15.,  ZMIN=-5.,ZMAX=5.,  YMIN=0.,YMAX=80. &END
/*
```

```
//*-------------------------------------------------------------------
//G.FT11F001 DD SYSOUT=*,DCB=(RECFM=UA,BLKSIZE=133)       SOURCE-MONITOR
//G.FT20F001 DD DSN=USER.REW031.BERTN,DISP=SHR            CASC-EVAP-DATA
//G.FT21F001 DD DSN=USRT.REW031.ELAS.TRG01,DISP=SHR
//G.FT10F001 DD DSN=USRT.REW031.NTRG01B,DISP=SHR
//G.FT30F001 DD DSN=USRT.REW031.HTRG01B,DISP=SHR
//G.FT40F001 DD DUMMY
//RELEASE EXEC RELEASE,JOBNAME=REW031T3,COND=(9,LT)
/* E O J
```

E.4 SIMPEL Analysis Input

```
//REW031T3 JOB (152,011881),STERZENBACH,TIME=(16),REGION=2000K,
//     CLASS=K,MSGCLASS=Y,TYPRUN=HOLD
/*JOBPARM  L=15
//*------->SUBMIT.S8.TRG01.TOTAL
//*------->SIMPEL   INTEGRAL PROPERTIES (EO=350.)
//SIM EXEC LGFORTE,COND=(9,LT)
//L.SYSPRINT DD DUMMY
//L.USER     DD DSN=USER.REW30LOD,DISP=SHR
//L.SYSIN    DD *
   INCLUDE USER(SIM008)
   ENTRY   MAIN
/*
//G.FT21F001 DD DSN=USER.REW031.O5RDAT(S8COM),DISP=SHR
//G.FT30F001 DD DSN=USRT.REW031.HTRG01B,DISP=SHR
//G.FT07F001 DD SYSOUT=*,DCB=(RECFM=UA,BLKSIZE=133)
//G.FT41F001 DD SYSOUT=*,DCB=(RECFM=UA,BLKSIZE=133)
//G.SYSIN    DD *
 C=' REFERENCE TARGET MIX.  INTEGRAL PROPERTIES';
 W=(0. 0. 0.);NORM=(0 0 0);MARG=(0 0 1 0 0 0);
 MED1=(1);MED2=(0);E=(1100. 350. 15. 0.);EQ=(1100. 350. 15.);
 DEFDET YNC,1,0,3,W,NORM,MARG,E,,MED1;
* CASCADE NEUTRON YIELD
 DEFDET YNE,2,0,3,W,NORM,MARG,E,,MED1;
* EVAPORATION NEUTRON YIELD
 DEFDET YPC,1,0,2,W,NORM,MARG,E,,MED1;
* CASCADE PROTON YIELD
 DEFDET YPE,2,0,2,W,NORM,MARG,E,,MED1;
* EVAPORATION PROTON YIELD
 DEFDET YPIC,1,0,15,W,NORM,MARG,E,,MED1;
* CASCADE PION YIELD
 DEFDET YMUC,1,0,16,W,NORM,MARG,E,,MED1;
* CASCADE MUON YIELD
 DEFDET YDE,2,0,9,W,NORM,MARG,E,,MED1;
* EVAPORATION DEUTERON YIELD
 DEFDET YTE,2,0,10,W,NORM,MARG,E,,MED1;
* EVAPORATION TRITON YIELD
 DEFDET YHE,2,0,11,W,NORM,MARG,E,,MED1;
* EVAPORATION HE-3 YIELD
 DEFDET YAE,2,0,12,W,NORM,MARG,E,,MED1;
* EVAPORATION ALPHA YIELD
 DEFDET QN,7,0,3,W,NORM,MARG,EQ,,MED1;
* NEUTRON FLUX
 DEFDET QP,7,0,2,W,NORM,MARG,EQ,,MED1;
```

```
* SECONDARY PROTON FLUX
 DEFDET QPI,7,0,15,W,NORM,MARG,EQ,,MED1;
* PION FLUX
 DEFDET QMU,7,0,16,W,NORM,MARG,EQ,,MED1;
* MUON FLUX
 DEFDET IN,5,0,3,W,NORM,MARG,EQ,,MED1,MED2;
* NEUTRON LEAKAGE CURRENT
 DEFDET IP,5,0,2,W,NORM,MARG,EQ,,MED1,MED2;
* PROTON LEAKAGE CURRENT
 DEFDET IPI,5,0,15,W,NORM,MARG,EQ,,MED1,MED2;
* PION LEAKAGE CURRENT
 DEFDET IMU,5,0,16,W,NORM,MARG,EQ,,MED1,MED2;
* MUON LEAKAGE CURRENT
 DEFDET DE,6,0,0,W,NORM,(0 0 1 0 0 0 ),,,MED1;
* ENERGY DEPOSITION
 SIMPEL 30,100;
 STOP;
/*
```

E.5 SIMPEL Primary Output

```
-------------------------------------------------------------------------------
C        = REFERENCE TARGET MIX.  INTEGRAL PROPERT
           IES
-------------------------------------------------------------------------------
W        (    3)=
  0.0              0.0              0.0
-------------------------------------------------------------------------------
NORM     (    3)=
           0          0          0
-------------------------------------------------------------------------------
MARG     (    6)=
           0          0          1          0          0
           0
-------------------------------------------------------------------------------
MED1     (    1)=
           1
-------------------------------------------------------------------------------
MED2     (    1)=
           0
-------------------------------------------------------------------------------
E        (    4)=
  1.100000E+03  3.500000E+02  1.500000E+01  0.0
-------------------------------------------------------------------------------
EQ       (    3)=
  1.100000E+03  3.500000E+02  1.500000E+01
-------------------------------------------------------------------------------
DEFDET NAME=YNC       TYP=    1 IOPT=    0 IPRT=    3
          W= 0.0          0.0          0.0
       NORM=            0            0            0
* CASCADE NEUTRON YIELD
E        (    4)=
  1.100000E+03  3.500000E+02  1.500000E+01  0.0
MED1     (    1)=
           1
```

```
DEFDET NAME=YNE       TYP=    2 IOPT=    0 IPRT=    3
          W= 0.0         0.0         0.0
        NORM=            0           0           0
* EVAPORATION NEUTRON YIELD
E       (    4)=
  1.100000E+03  3.500000E+02  1.500000E+01  0.0
MED1    (    1)=
         1
```

```
DEFDET NAME=YPC       TYP=    1 IOPT=    0 IPRT=    2
          W= 0.0         0.0         0.0
        NORM=            0           0           0
* CASCADE PROTON YIELD
E       (    4)=
  1.100000E+03  3.500000E+02  1.500000E+01  0.0
MED1    (    1)=
         1
```

```
DEFDET NAME=YPE       TYP=    2 IOPT=    0 IPRT=    2
          W= 0.0         0.0         0.0
        NORM=            0           0           0
* EVAPORATION PROTON YIELD
E       (    4)=
  1.100000E+03  3.500000E+02  1.500000E+01  0.0
MED1    (    1)=
         1
```

```
DEFDET NAME=YPIC      TYP=    1 IOPT=    0 IPRT=   15
          W= 0.0         0.0         0.0
        NORM=            0           0           0
* CASCADE PION YIELD
E       (    4)=
  1.100000E+03  3.500000E+02  1.500000E+01  0.0
MED1    (    1)=
         1
```

```
DEFDET NAME=YMUC      TYP=    1 IOPT=    0 IPRT=   16
          W= 0.0         0.0         0.0
        NORM=            0           0           0
* CASCADE MUON YIELD
E       (    4)=
  1.100000E+03  3.500000E+02  1.500000E+01  0.0
MED1    (    1)=
         1
```

```
DEFDET NAME=YDE       TYP=    2 IOPT=    0 IPRT=    9
          W= 0.0         0.0         0.0
        NORM=            0           0           0
* EVAPORATION DEUTERON YIELD
E       (    4)=
  1.100000E+03  3.500000E+02  1.500000E+01  0.0
MED1    (    1)=
         1
```

```
DEFDET NAME=YTE       TYP=    2 IOPT=    0 IPRT=   10
          W= 0.0         0.0         0.0
       NORM=           0           0           0
* EVAPORATION TRITON YIELD
E       (    4)=
  1.100000E+03  3.500000E+02  1.500000E+01  0.0
MED1    (    1)=
         1
```

```
DEFDET NAME=YHE       TYP=    2 IOPT=    0 IPRT=   11
          W= 0.0         0.0         0.0
       NORM=           0           0           0
* EVAPORATION HE-3 YIELD
E       (    4)=
  1.100000E+03  3.500000E+02  1.500000E+01  0.0
MED1    (    1)=
         1
```

```
DEFDET NAME=YAE       TYP=    2 IOPT=    0 IPRT=   12
          W= 0.0         0.0         0.0
       NORM=           0           0           0
* EVAPORATION ALPHA YIELD
E       (    4)=
  1.100000E+03  3.500000E+02  1.500000E+01  0.0
MED1    (    1)=
         1
```

```
DEFDET NAME=QN        TYP=    7 IOPT=    0 IPRT=    3
          W= 0.0         0.0         0.0
       NORM=           0           0           0
* NEUTRON FLUX
EQ      (    3)=
  1.100000E+03  3.500000E+02  1.500000E+01
MED1    (    1)=
         1
```

```
DEFDET NAME=QP        TYP=    7 IOPT=    0 IPRT=    2
          W= 0.0         0.0         0.0
       NORM=           0           0           0
* SECONDARY PROTON FLUX
EQ      (    3)=
  1.100000E+03  3.500000E+02  1.500000E+01
MED1    (    1)=
         1
```

```
DEFDET NAME=QPI       TYP=    7 IOPT=    0 IPRT=   15
          W= 0.0         0.0         0.0
       NORM=           0           0           0
* PION FLUX
EQ      (    3)=
  1.100000E+03  3.500000E+02  1.500000E+01
MED1    (    1)=
         1
```

```
-----------------------------------------------------------------
DEFDET NAME=QMU       TYP=   7 IOPT=   0 IPRT=  16
          W= 0.0         0.0         0.0
        NORM=            0           0           0
* MUON FLUX
EQ       (   3)=
  1.100000E+03  3.500000E+02  1.500000E+01
MED1     (   1)=
         1
-----------------------------------------------------------------
DEFDET NAME=IN        TYP=   5 IOPT=   0 IPRT=   3
          W= 0.0         0.0         0.0
        NORM=            0           0           0
* NEUTRON LEAKAGE CURRENT
EQ       (   3)=
  1.100000E+03  3.500000E+02  1.500000E+01
MED1     (   1)=
         1
MED2     (   1)=
         0
-----------------------------------------------------------------
DEFDET NAME=IP        TYP=   5 IOPT=   0 IPRT=   2
          W= 0.0         0.0         0.0
        NORM=            0           0           0
* PROTON LEAKAGE CURRENT
EQ       (   3)=
  1.100000E+03  3.500000E+02  1.500000E+01
MED1     (   1)=
         1
MED2     (   1)=
         0
-----------------------------------------------------------------
DEFDET NAME=IPI       TYP=   5 IOPT=   0 IPRT=  15
          W= 0.0         0.0         0.0
        NORM=            0           0           0
* PION LEAKAGE CURRENT
EQ       (   3)=
  1.100000E+03  3.500000E+02  1.500000E+01
MED1     (   1)=
         1
MED2     (   1)=
         0
-----------------------------------------------------------------
DEFDET NAME=IMU       TYP=   5 IOPT=   0 IPRT=  16
          W= 0.0         0.0         0.0
        NORM=            0           0           0
* MUON LEAKAGE CURRENT
EQ       (   3)=
  1.100000E+03  3.500000E+02  1.500000E+01
MED1     (   1)=
         1
MED2     (   1)=
         0
```

```
-------------------------------------------------------------------
DEFDET NAME=DE        TYP=    6 IOPT=    0 IPRT=    0
          W= 0.0         0.0          0.0
       NORM=            0            0           0
* ENERGY DEPOSITION
MED1     (    1)=
          1
-------------------------------------------------------------------

SUBMIT=SUBMIT.HETN.TRG01B
NTPNAM= 3
NTPMAX= 1
BATCH #  1  COMPLETED
BATCH #  2  COMPLETED
BATCH #  3  COMPLETED

      and so on

BATCH # 97  COMPLETED
BATCH # 98  COMPLETED
BATCH # 99  COMPLETED
BATCH #100  COMPLETED

Y(E,A,R)   CASC.
REGION=  1.000
           I                        I
-------------------------------------------------------------------
 3.500E+02 I  0.0         :    0.0  I
 1.500E+01 I  5.435E-01   :    1.98 I
 0.0       I  6.101E-01   :    1.80 I
-------------------------------------------------------------------

* CASCADE NEUTRON YIELD
Y(R)       CASC.
           I                        I
-------------------------------------------------------------------
   1       I  1.154E+00   :    1.67 I
-------------------------------------------------------------------
TOTAL DETECTOR RESPONSE   : 1.1535959E+00  F.S.D.: 1.6718227E-02
TOTAL NO. OF CONTRIBUTION: 1.1535997E+00  F.S.D.: 1.6717918E-02

* EVAPORATION NEUTRON YIELD
Y(E,A,R)   EVAP.
REGION=  1.000
           I                        I
-------------------------------------------------------------------
 3.500E+02 I  0.0         :    0.0  I
 1.500E+01 I  9.900E-03   :    9.89 I
 0.0       I  4.856E+00   :    1.60 I
-------------------------------------------------------------------

* EVAPORATION NEUTRON YIELD
Y(R)       EVAP.
           I                        I
-------------------------------------------------------------------
   1       I  4.866E+00   :    1.60 I
```

```
TOTAL DETECTOR RESPONSE  : 4.8662663E+00  F.S.D.: 1.5969515E-02
TOTAL NO. OF CONTRIBUTION: 4.8662996E+00  F.S.D.: 1.5969783E-02

* CASCADE PROTON YIELD
Y(E,A,R)   CASC.
REGION=  1.000
           I                        I
-------------------------------------------------------------------
 3.500E+02 I  0.0        :    0.0  I
 1.500E+01 I  3.903E-01  :    1.85 I
 0.0       I  2.520E-02  :    7.01 I
-------------------------------------------------------------------

* CASCADE PROTON YIELD
Y(R)       CASC.
           I                        I
-------------------------------------------------------------------
   1       I  4.155E-01  :    1.82 I
-------------------------------------------------------------------
TOTAL DETECTOR RESPONSE  : 4.1549760E-01  F.S.D.: 1.8242884E-02
TOTAL NO. OF CONTRIBUTION: 4.1549999E-01  F.S.D.: 1.8242784E-02

* EVAPORATION PROTON YIELD
Y(E,A,R)   EVAP.
REGION=  1.000
           I                        I
-------------------------------------------------------------------
 3.500E+02 I  0.0        :    0.0  I
 1.500E+01 I  2.800E-03  :   18.36 I
 0.0       I  8.080E-02  :    4.59 I
-------------------------------------------------------------------

* EVAPORATION PROTON YIELD
Y(R)       EVAP.
           I                        I
-------------------------------------------------------------------
   1       I  8.360E-02  :    4.56 I
-------------------------------------------------------------------
TOTAL DETECTOR RESPONSE  : 8.3599985E-02  F.S.D.: 4.5572393E-02
TOTAL NO. OF CONTRIBUTION: 8.3599985E-02  F.S.D.: 4.5572393E-02

* CASCADE PION YIELD
Y(E,A,R)   CASC.
REGION=  1.000
           I                        I
-------------------------------------------------------------------
 3.500E+02 I  0.0        :    0.0  I
 1.500E+01 I  2.299E-03  :   22.14 I
 0.0       I  1.400E-03  :   28.75 I
-------------------------------------------------------------------

* CASCADE PION YIELD
Y(R)       CASC.
           I                        I
-------------------------------------------------------------------
   1       I  3.699E-03  :   17.45 I
```

```
TOTAL DETECTOR RESPONSE  : 3.6989683E-03  F.S.D.: 1.7451954E-01
TOTAL NO. OF CONTRIBUTION: 3.6999998E-03  F.S.D.: 1.7458540E-01

* CASCADE MUON YIELD
>>> NO CONTRIBUTIONS FOUND FOR THIS DETECTOR <<<

* EVAPORATION DEUTERON YIELD
Y(E,A,R)   EVAP.
REGION=  1.000
           I                        I
-----------------------------------------------------------------
 3.500E+02 I  0.0        :   0.0  I
 1.500E+01 I  2.400E-03  :  19.75 I
 0.0       I  4.320E-02  :   5.36 I
-----------------------------------------------------------------

* EVAPORATION DEUTERON YIELD
Y(R)       EVAP.
           I                        I
-----------------------------------------------------------------
   1       I  4.560E-02  :   5.45 I
-----------------------------------------------------------------
TOTAL DETECTOR RESPONSE  : 4.5599997E-02  F.S.D.: 5.4462291E-02
TOTAL NO. OF CONTRIBUTION: 4.5599997E-02  F.S.D.: 5.4462291E-02

* EVAPORATION TRITON YIELD
Y(E,A,R)   EVAP.
REGION=  1.000
           I                        I
-----------------------------------------------------------------
 3.500E+02 I  0.0        :   0.0  I
 1.500E+01 I  6.100E-03  :  12.53 I
 0.0       I  4.790E-02  :   4.55 I
-----------------------------------------------------------------

* EVAPORATION TRITON YIELD
Y(R)       EVAP.
           I                        I
-----------------------------------------------------------------
   1       I  5.400E-02  :   4.36 I
-----------------------------------------------------------------
TOTAL DETECTOR RESPONSE  : 5.3997874E-02  F.S.D.: 4.3569867E-02
TOTAL NO. OF CONTRIBUTION: 5.3999998E-02  F.S.D.: 4.3567438E-02

* EVAPORATION HE-3 YIELD
Y(E,A,R)   EVAP.
REGION=  1.000
           I                        I
-----------------------------------------------------------------
 3.500E+02 I  0.0        :   0.0  I
 1.500E+01 I  1.000E-04  : 100.00 I
 0.0       I  3.000E-04  :  57.15 I
-----------------------------------------------------------------

* EVAPORATION HE-3 YIELD
Y(R)       EVAP.
           I                        I
```

```
-------------------------------------------------------------------
   1       I  4.000E-04 :  49.24 I
-------------------------------------------------------------------
TOTAL DETECTOR RESPONSE   : 3.9999979E-04  F.S.D.: 4.9236590E-01
TOTAL NO. OF CONTRIBUTION: 3.9999979E-04  F.S.D.: 4.9236590E-01

* EVAPORATION ALPHA YIELD
Y(E,A,R)   EVAP.
REGION=  1.000
           I                        I
-------------------------------------------------------------------
 3.500E+02 I  0.0       :   0.0  I
 1.500E+01 I  7.370E-02 :   3.76 I
 0.0       I  1.990E-02 :   8.25 I
-------------------------------------------------------------------

* EVAPORATION ALPHA YIELD
Y(R)       EVAP.
           I                        I
-------------------------------------------------------------------
   1       I  9.360E-02 :   3.58 I
-------------------------------------------------------------------
TOTAL DETECTOR RESPONSE   : 9.3596697E-02  F.S.D.: 3.5823721E-02
TOTAL NO. OF CONTRIBUTION: 9.3599975E-02  F.S.D.: 3.5822030E-02

* NEUTRON FLUX
PHI.V(E,A,R)
REGION=  1.000
           I                        I
-------------------------------------------------------------------
 3.500E+02 I  0.0       :   0.0  I
 1.500E+01 I  3.858E+00 :   2.16 I
-------------------------------------------------------------------

* NEUTRON FLUX
PHI.V(R)
           I                        I
-------------------------------------------------------------------
   1       I  3.858E+00 :   2.16 I
-------------------------------------------------------------------
TOTAL DETECTOR RESPONSE   : 3.8581972E+00  F.S.D.: 2.1643110E-02
TOTAL NO. OF CONTRIBUTION: 6.9959998E-01  F.S.D.: 2.0579584E-02

* SECONDARY PROTON FLUX
PHI.V(E,A,R)
REGION=  1.000
           I                        I
-------------------------------------------------------------------
 3.500E+02 I  0.0       :   0.0  I
 1.500E+01 I  3.951E-01 :   2.61 I
-------------------------------------------------------------------

* SECONDARY PROTON FLUX
PHI.V(R)
           I                        I
-------------------------------------------------------------------
   1       I  3.951E-01 :   2.61 I
```

```
TOTAL DETECTOR RESPONSE   : 3.9505094E-01  F.S.D.: 2.6098087E-02
TOTAL NO. OF CONTRIBUTION: 4.0329999E-01  F.S.D.: 1.8937878E-02

* PION FLUX
PHI.V(E,A,R)
REGION=  1.000
          I                        I
-----------------------------------------------------------------
 3.500E+02 I  0.0        :   0.0  I
 1.500E+01 I  1.241E-03  :  33.37 I
-----------------------------------------------------------------

* PION FLUX
PHI.V(R)
          I                        I
-----------------------------------------------------------------
   1      I  1.241E-03  :  33.37 I
-----------------------------------------------------------------
TOTAL DETECTOR RESPONSE   : 1.2414369E-03  F.S.D.: 3.3365566E-01
TOTAL NO. OF CONTRIBUTION: 1.4999998E-03  F.S.D.: 2.7421945E-01

* MUON FLUX
PHI.V(E,A,R)
REGION=  1.000
          I                        I
-----------------------------------------------------------------
 3.500E+02 I  0.0        :   0.0  I
 1.500E+01 I  9.454E-07  :  88.01 I
-----------------------------------------------------------------

* MUON FLUX
PHI.V(R)
          I                        I
-----------------------------------------------------------------
   1      I  9.454E-07  :  88.01 I
-----------------------------------------------------------------
TOTAL DETECTOR RESPONSE   : 9.4535756E-07  F.S.D.: 8.8008648E-01
TOTAL NO. OF CONTRIBUTION: 1.9999999E-04  F.S.D.: 7.0352632E-01

* NEUTRON LEAKAGE CURRENT
J(E,A,S)
REGION=  1.000
          I                        I
-----------------------------------------------------------------
 3.500E+02 I  0.0        :   0.0  I
 1.500E+01 I  2.405E-01  :   2.10 I
-----------------------------------------------------------------

* NEUTRON LEAKAGE CURRENT
J(S)
          I                        I
-----------------------------------------------------------------
     1.000 I  2.405E-01  :   2.10 I
-----------------------------------------------------------------
TOTAL DETECTOR RESPONSE   : 2.4049783E-01  F.S.D.: 2.1045011E-02
TOTAL NO. OF CONTRIBUTION: 2.4049997E-01  F.S.D.: 2.1044623E-02
```

```
* PROTON LEAKAGE CURRENT
J(E,A,S)
REGION=  1.000
          I                        I
-------------------------------------------------------------------
 3.500E+02 I  0.0        :    0.0  I
 1.500E+01 I  1.600E-03  :   24.68 I
-------------------------------------------------------------------

* PROTON LEAKAGE CURRENT
J(S)
          I                        I
-------------------------------------------------------------------
     1.000 I  1.600E-03  :   24.68 I
-------------------------------------------------------------------
TOTAL DETECTOR RESPONSE  : 1.5999998E-03  F.S.D.: 2.4682307E-01
TOTAL NO. OF CONTRIBUTION: 1.5999998E-03  F.S.D.: 2.4682307E-01

* PION LEAKAGE CURRENT
>>> NO CONTRIBUTIONS FOUND FOR THIS DETECTOR <<<

* MUON LEAKAGE CURRENT
>>> NO CONTRIBUTIONS FOUND FOR THIS DETECTOR <<<
```

E.6 SIMPEL Secondary Output (ECHO unit)

```
C=' REFERENCE TARGET MIX.  INTEGRAL PROPERTIES';
W=(0. 0. 0.);NORM=(0 0 0);MARG=(0 0 1 0 0 0);
MED1=(1);MED2=(0);E=(1100. 350. 15. 0.);EQ=(1100. 350. 15.);
DEFDET YNC,1,0,3,W,NORM,MARG,E,,MED1;
DEFDET YNE,2,0,3,W,NORM,MARG,E,,MED1;
DEFDET YPC,1,0,2,W,NORM,MARG,E,,MED1;
DEFDET YPE,2,0,2,W,NORM,MARG,E,,MED1;
DEFDET YPIC,1,0,15,W,NORM,MARG,E,,MED1;
DEFDET YMUC,1,0,16,W,NORM,MARG,E,,MED1;
DEFDET YDE,2,0,9,W,NORM,MARG,E,,MED1;
DEFDET YTE,2,0,10,W,NORM,MARG,E,,MED1;
DEFDET YHE,2,0,11,W,NORM,MARG,E,,MED1;
DEFDET YAE,2,0,12,W,NORM,MARG,E,,MED1;
DEFDET QN,7,0,3,W,NORM,MARG,EQ,,MED1;
DEFDET QP,7,0,2,W,NORM,MARG,EQ,,MED1;
DEFDET QPI,7,0,15,W,NORM,MARG,EQ,,MED1;
DEFDET QMU,7,0,16,W,NORM,MARG,EQ,,MED1;
DEFDET IN,5,0,3,W,NORM,MARG,EQ,,MED1,MED2;
DEFDET IP,5,0,2,W,NORM,MARG,EQ,,MED1,MED2;
DEFDET IPI,5,0,15,W,NORM,MARG,EQ,,MED1,MED2;
DEFDET IMU,5,0,16,W,NORM,MARG,EQ,,MED1,MED2;
DEFDET DE,6,0,0,W,NORM,(0 0 1 0 0 0 ),,,MED1;
SIMPEL 30,100;
STOP;
```