Manual for Code Alice version July 7,2008*

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1 Introduction

This is the revision of a user manual for the nuclear reactions code Alice . The Monte Carlo version will be described. It is based on the HMS precompound decay (1), Weisskopf-Ewing evaporation (2), and Bohr- Wheeler (3) fission models. Treatment of angular distributions uses the linear momentum conservation model of Chadwick and Oblozinsky (4). The code is intended to be relatively fast in execution and easy to use.The ease of use is facilitated by several library files which must be present at time of execution, internal data files, and subroutines to prepare data necess- ary for the calculations.

In Sect. 2 we present a description/examples of running the code, along with a description of options which may be invoked at user discretion. In Sect. 3 we describe the library files necessary for execution and sources of those data, as well as some of the internal data/parameter sources. In Sect. 4 we describe some of the physical models/assumptions used in different aspects of code execution.

The present code version accepts incident particles of photons, neutrons protons, and heavy ions, e.g.^4He and heavier. Earlier versions also accepted stopped pions. Targets from Be up are possible, though light elements can present problems for trust in results. Incident energies of 0.2 - 250 MeV are acceptable. In point of fact, excitations below 1 GeV are tolerated; lack of pion production/decay treatment raises questions as to the judgement in application above 250 MeV.

The organization of this report is to facilitate a user whose first interest may be to 'just run the code', without getting bogged down in a discussion of the physics. The latter is therefore presented in later sections. * refer questions to M.Blann, blann@verizon.net

2 Code execution and options

In this sect. we will write screen interrogation of user in all caps, and possible responses in lower case for title, numbers for those to be entered. A number will be placed in parentheses identifying the 7 lines the user will input for example 1.These numbers are not to be entered-they are only to permit reference to input lines.Comments not to be entered will be in parenthesis.

2.1 Example 1: Default options

We present a calculation of neutrons on U235 at incident energies of 2 to 18 Mev in 2 MeV increments, with 20,000 MC events run at each energy.

The user will first be prompted to enter a 0 (zero) to execute from an existing file INSAVE, or enter a 1 (one) to enter input from screen. Better the latter for first use (the file entered will be saved as INSAVE for later use if desired). Therefore after activating the code by entering ALICE.x (or on some systems './ALICE.x'), enter:

(1) 1(return)(note: this will cause screen interrogation for additional input)

ENTER TITLE LINE TO IDENTIFY THIS PROBLEM NOW

(2) test case of neutrons on U235 at 2-18 Mev example (enter)

ENTER 4 VALUES ON THE NEXT LINE
ZP THE PROJECTILE ATOMIC NUMBER
AP THE PROJECTILE MASS NUMBER
ZT " TARGET ATOMIC NUMBER
ZP " " MASS NO

ENTER THESE 4 VALUES NOW

(3) 0 1 92 235 (enter)

(4) ENTER THE ENERGY (HISTOGRAM) MESHSIZE (MeV) AND THE NUMBER OF EVENTS FOR THE MONTE CARLO CALCULATION.

ED
NCOUNT

0.2 20000 (Here we use a 0.2 MeV meshsize and will run 20000 cascade events at each incident energy.)

THE NEXT ENTRIES CONTROL PROJECTILE ENERGIES: THERE ARE TWO POSS IBLE MODES; EITHER A LIST OF ENERGIES TO BE USED, OR A LOOP OF "NENG" ENERGIES FOR WHICH THE FIRST ENERGY "EINC" IS GIVEN (LAB FRAME) FOLLOWED BY THE INCREMENT IN ENERGY "EDELT". THE CHOICE IS MADE BY ENTERING

NENG AS A NEGATIVE NUMBER (LIST OF ENERGIES), OR AS A POSITIVE NUMBER (LOOP ON EDELT)

IN EITHER CASE,THERE IS A LIMIT OF 100 ENERGIES PER PROBLEM. ENTER NENG ON THE NEXT LINE NOW

(5) 9 (enter)

ENTER THE FIRST ENERGY EINC AND EDELT, THE LOOP INCREMENT NOW

(6) 2 2 (note: if we had entered "-9" for NENG, we would here enter any 9 energies we wished to have calculated; by the choice we made, the calculation will be run for incident neutron energies of 2,4,6,8,10,12,14,16,18 MeV)

ISTART TO BEGIN EXECUTION OF THIS PROBLEM, ENTER "777" TO VIEW OPTIONS TO CHANGE SOME DEFAULT PARAMETERS, TYPE "333"

(7) 777 (enter)

Congratulations! The calculation should now be underway.

Note that your input file has been saved as 'insave'. You may wish to give it a descriptive name to save it in case you decide to re-run this calculation changing some parameter such as number of events,target,projectile, energy mesh size, etc. To do so, you may edit

the changes into the 'insave' file, then re-run the code entering a "0" for the first entry (line [1], and the edited insave file will be used to run the code.

OUTPUT FILES

The following screen output should follow completion of the calculation:
' Calculation is completed;the following output files have been created:'
"INSAVE " input file created from screen input'
' "OUTPT" many things-read to check-may reduce in future'
' "PLOT " contains excitation function plots'(note: for spallation yields;fission yields are in the following 4 files. Isomer yields/ratios are included in the plot file)
' "FOUT" fission product yields vs. incident energy
' "FIZISOMR" fission product yields'
' "FIZISRAT" fission isomer ratios '
' "FIZYBYA" fission mass yields '
' "FRAGSS" fission fragment distributions:mass vs Z,' ' and Z yields for fixed A'
' "FIZYLDS" fission fragment yields with normalization'
(note: the following output files are for the n,p,alpha emissions. Should the parameter 'limout',option have been entered as '1' rather than zero, this output message would end at this point-the spectral arrays would not be printed)
' "SDCSCM" single differential cross sections in CM frame (mb/MeV)
' "LABOUT" single differential cross sections in LAB frame (mb/MeV)
' "ENGANG" energy columns versus angle DDCS in CM frame (mb/Mev/sr)'
' "ANGENG" angle columns versus energy in CM frame (mb/MeV/sr)
' "LABANGD" DDCS in LAB frame angle columns vs. energy (mb/MeV/sr)'
' "LABENGD" DDCS in LAB frame,energy columns vs. angle (mb/MeV/sr)'
' "SDCSFLB" single diff. fission fragment emitted n,p,alpha spectra' ' in LAB frame (mb/Mev*sr)'
' "SDCSFCM" single differential particle spectra in' ' fission fragment frame (not true cm)'
' "SDCSTOTLB" total single differential spectra,evap.' ' plus fission n,p,alpha,LAB frame'
' "DDCSFLB" double diff. spectra of n,p,alpha emitted from fission frags.' ' in LAB frame,angle vs energy'
' "DDCSFCM" double diff. fission part. spectra' ' in ff frame,energy vs. angle'
' "DDCSTOTLB" total double differential spectra for' ' fission+evaporation n,p,alpha,LAB frame'

2.2 Example 2: Other than default options

We present the whole screen interactive session below for the case of protons on Holmium 165 with some special options selected.We separate editorial comments from the session results by parentheses. Screen output:

Welcome to Alice"s Wonderland 2008
This version by W.B.Wilson(LANL,Ret.,
S.G.Mashnik,(LANL),A.Konobeyev (Karls-
ruhe) and M.Blann

version March 2008 Note fission LD parms need adjustment, gamma spectra have not been benchmarked. ENDV output have been set only up to 3 particles out exclusive.

Follow the screen directions to avoid a bad hare day.
Unless otherwise stated,all formats are free format.
To read a standard file "INSAVE" enter "0" now,
or for input via SCREEN PROMPT,enter "1" now.
This code version requires library files phtlib, tmadland,MASS.TBL,SHELL.TBL,pmtable,gdrparms for execution

1 (entered to select screen interrogation input)

Enter a title line to identify this problem

protons +165Ho (this is a title line)
Enter 4 values on the next line :
ZP the projectile atomic no.

AP " " mass no.

ZT the target atomic no.

AT " " mass no.(use 1000 for isotopic targets- not yet available HI projectiles)

note that zp=ap=0 is interpreted as a photon

1 1 67 165 (here we enter projectile and target identification)

make two entries on the next line:

ED the ejectile channel energy histogram width (this should be an integer increment of 0.1 MeV;e.g. 0.1,0.5,etc. If you enter 0, default will be 0.5 MeV

NCOUNT Number of cascades to run for MC option if "0" is entered,default is 100000 events

0.2 10000 (we want to use a histogram meshsize of 0.2 MeV and run 10000 events each energy)

The next entries control projectile energies:there are TWO possible modes;either a list of energies to be used,or a loop of "NENG" energies,for which the first energy "EINC" is given(lab frame),followed by the increment in energy, EDELT.The choice is made by entering

"NENG" as a negative number (list of energies),or as a positive number(loop on EDELT).

In either case,there is a limit of 100 energies per problem

Enter NENG now

-2 (we will run 2 energies, and we will specify each)

Enter a list of 2 incident energies EINC

50 100 (energies selected will be 50 and 100 MeV incident protons)

To begin execution of this problem, ENTER "777"
To re-enter data, ENTER "111"
To view options to change default parms, ENTER "333"

333 (we want to see all options available rather than the default to alice's choices)

Default options may be changed by inputting a number which is a sum of "PARM" integers as follows:

for ENDV output PARM=256

for emission of d,t,3He and 7Be in addition to default n,p,4He (precompound+evaporation),PARM=128

for user provided reaction cross sections, PARM= 64

for inverse cross section options, PARM= 32

ALICE selects level densities as Fermi gas or Kataria-Ramamurthy based on shell proximity;to force a choice, including Obninsk densities, PARM= 16

for an isomeric,rather than gstate target PARM= 8

to use the s-wave angular momentum approx PARM= 4

To limit output to yields /suppress spectra, PARM= 1

Enter the sum of all PARM values (as integer)for options you wish to select

144 (We choose to allow precompound emission of d,t,3He and 7Be in addition to the default n,p,4He, and to force choice of level density options.Had we wished e.g. ENDV output as well, we would have entered 400 rather than 144. Some options will bring up additional menus.)

Default is to select Fermi gas or Kataria level densities internally. Other options are as follows:

The next line has two entries:

LDOPT level density option: 0 Fermi gas,backshifted pairing energies 1 Kataria-Ramamurthy 2 Obninsk (note fission not working with thi s option) 3 Gilbert -Cameron, not yet tested 6 uses calculated liquid drop masses with neither shell nor pairing terms

PLD enter FG level density parameter here,or "0" for default "9",i.e. a=A/9

Enter these two values now

0 0 (We have elected to insist on Fermi gas level densities, with default a=A/9/ level density parameter, rather than allowing Alice to select the level density model based on shell structure near the composite nucleus)

(below lines give a progress report as calculation progresses) 0

zee,amass,nz,na,mc,mp,ap,at,zp,zt 68.00000 166.0000 13 22 10 1 1.000000 165.0000 1.000000 67.00000 1 now doing energy = 50.00000 MeV monte carlo precompound option selected;no. events = 10000

now doing energy = 100.0000 MeV monte carlo precompound option selected;no. events = 10000

(below is a listing of the output files; the number of files listed will depend somewhat on the choice of parameters, projectile..)

Calculation is completed;the following output files h ave been created:

"INSAVE " input file created from screen input

"OUTPT" many things-read to check-may reduce in future

"PLOT " contains excitation function data for plots

"FOUT" fission product yields-A,Excitation,Z

"FIZISOMR" fission product yields

"FIZISRAT" fission isomer ratios

"FIZYBYA" fission mass yields

"FRAGSS" fission fragment distributions:mass vs Z, and Z yields for fixed A

"FIZYLDS" fission fragment yields with normalization

"SDCSCM" single differential cross sections in CM frame (mb/MeV)

"ENGANG" energy columns versus angle DDCS in CM frame(mb/MeV/sr)

"ANGENG" angle columns versus energy in CM frame(mb/ MeV/sr)

"SDCSTOTLB" total single differential spectra,evap. plus fission n,p,alpha,LAB frame

"LABOUT" single differential cross sections in LAB frame (mb/MeV)

"LABANGD" DDCS in LAB frame angle columns vs. energy (mb/MeV/sr)

"LABENGD" DDCS in LAB frame,energy columns vs. angle (mb/MeV/sr)

"SDCSFLB" single diff. fission fragment emitted n,p,alpha spectra in LAB frame (mb/Mev*sr)

"SDCSFCM" single differential particle spectra in fission fragment frame (not true cm) plus fission n,p,alpha,LAB frame

"DDCSFLB" double diff. spectra of n,p,alpha emitted from fission fragments in LAB frame,A vs E

"DDCSFCM" double diff. fission part. spectra in ff frame,energy vs. angle

"DDCSTOTLB" total double differential spectra for fission+evaporation n,p,alpha,LAB frame

"SDCSCL " single differential cross section clusters from evaporation process, cm frame

"SDLBCL " single differential cross section clusters from evaporation process, lab frame

"GAMMASPEC" gamma ray spectra summed over nuclides

DAS IST ALICE DAS IST ALICE DAS IST ALICE DAS IST ALICE DAS IST ALICE

(The line above means that the code has completed and made a normal exit; it has historical reasons for existence. The alice code started at Univ. of Rochester in 1962 on an IBM 650 computer with 2000 words of memory, not all useable. Square roots took 11 ms. to compute, so it may be seen that the code development has depended on technological evolution, as well as progress in understanding nuclear physics).

(below we offer a few other examples of use of parameter options)

If you used a 64 in your sum, you will be prompted to enter your own reaction cross sections:

if(ireact.gt.0.and.neng.lt.0)then Now enter ',nengg,' reaction cross sections in the same order as the incident energies endif

if(ireact.gt.0.and.neng.ge.0)then
write(*,*)' Enter ',neng,'reaction cross sections,one for each write(*,*)' incident energy,starting with EINC endif

If you added a value of "32" to your parm input, you will be asked to select your choice of inverse reaction cross sections:

INVER inverse reaction cross section option
"0" selects the nuclear optical model;
"2" selects the classical sharp cutoff
(faster but less accurate)

If you added a "16" to your PARM, you will be given a menu of level density options from which to choose.Initially these will be only Fermi gas and the Kataria-Ramamurthy shell corrected models- but keep checking as new choices will be added.

Default is to select Fermi gas or Kataria level densities internally. Other options are as follows:

The next line has two entries:

LDOPT level density option:
0 Fermi gas,backshifted pairing energie
1 Kataria-Ramamurthy

PLD enter FG level density parameter here,or
"0" for default "9",i.e. a=A/9

Enter these two values now

If the PARM parameter has a value of "8" added to it, you have elected to use an isomer as target rather than the ground state:

LEVNO Isomers may be used as targets; for ground state target enter "0", for m1 "1", for m2 "2"

If you added a value of "4" to PARM, you may select the "s-wave" approximation in which all angular momentum is assumed to be in rotational energy:

IROTOR enter "0" for no rotational energy correction, or "1" for the "s-wave approximation"

If you added "2" to PARM, you will be given options on treating heavy ion reactions (A¿3):

ICOUPLE For heavy ion reactions (mass projectile gt 1.), actual coupling of Fermi energies may be selected rather than a faster algorithm,and the default Fermi energies

of target and projectile may be changed from the 35 MeV values. Enter the following parameters, or enter zeroes for default:

enter ICOUPLE as "1" to use the algorithm for DDCS,or"0" for actual random coupling of Fermi momenta

enter EFERMT,EFERMP target and projectile Fermi energies Enter these values now, or "0" for default 35 MeV

If a "1" was added to PARM, you have elected to choose to limit output to yields only, no spectra:

LIMOUT enter limout as "1" to limit output to yield files only,

CAUTION ON INPUT PARAMETERS

Arrays for particle spectra and residual nucleus excitations have a dimension limit of 999. It is not recommended to use the code above incident energies of around 200 MeV. The user must use caution when selecting the energy mesh size parameter ED so as not to exceed the bounds of these arrays. A rule is that maximum incident energy plus 10 divided by ED should not exceed 999. Thus to use an incident energy of 200 MeV with ed=0.2 would be dangerous. If the smaller mesh size was desired for accuracy, it would be better to divide the calculation into two sets, one at energies below 190 with the smaller mesh size,the second above 190 with, e.g a 0.5 MeV mesh. The code is designed to skip to the next incident energy if the excitation/mesh size ratio is near the dimension limit.

In choosing inverse reaction cross sections, the option INVER=2 uses a classical sharp cutoff algorithm in subroutine sigi to give reasonably good numbers very quickly. The option INVER=0 uses the nuclear optical model. It is the preferred choice, but takes a little longer. In using a MC code to good statistics, the time difference is likely a negligible fraction of the run time.

3 Running with PREALICE

Presently the code is sometimes run with a driver, PREALICE written by M.B.Chadwick and W.B.Wilson at LANL.The driver makes input files for diff- erent Z,A targets. At present it always runs 44 incident energies, and supplies the reaction cross section at each energy using fast algorithms. If the code is run with the driver, we presently set a parameter IMSG=1, then a parameter MASTERPARM is offered; if it is selected with a "0" value, the following parameters are set internally without further interrogation: LIMOUT=1 ED= 0.2 ISOT=1 IPARM=0 JCAL=1 IREACT=1 PLD=9 M3=3 INVER=0 MCEVA=4 KINEM=1 NENG= -44 IGATE=0 CLD=1.02 The last two of these parameters are overridden later or not used. To modify the Alice code to run with this driver,comment designations need to be removed from 2 lines around 641:

c inopt=0 c imsg=1

4 Library files, data files and parameters from within

Library files which must be in the accessible file system:

PHTLIB (FILE 28)2641 lines. For a list of isotopes, this file gives the spins and parities of ground and isomeric states. It also gives the energies of isomeric states. It identifies if the values are from the nuclear data tables, or have been guessed from properties of neighboring isotopes. These data are used to determine which nuclides have isomers, and their energies and spins are used in estim- ating isomer yields. Estimates are based on the Huizenga- Vandenbosch model (5).

TMADLAND (FILE 30)68 lines. This lists primary fission barrier heights deduced from various sources by D.G.Madland, and generously provided for use with Alice via private communication, Nov.1, 2002. Isotopes covered range from Z88/A228 to Z99/A251.These data are used for ground state fission barriers. For all other isotopes, barriers are taken from the mass formula of P.Moller (6). Then all barriers are scaled with angular momentum using the Moller rotating finite range mass model, multiplying by the barrier at ground state to that at spin J.

GDRPARMS (FILE 38)5986 lines.This file provides the parameters for calculating a double Lorentzian GDR capture cross section for incident photons.It replaces an earlier Berman-Fultz parameterization. The cross section also includes a quasi-deuteron contribution with formulation due to M.B. Chadwick. Details of the capture cross section calculation may be found in subroutine photin. The parameter file was provided by Dr. Marie Giacri/Saclay, private comm. Oct. 2004. Values were from S.Goriely,M.Pearson and F.Tondeur.

MASS.TBL (FILE 31)9796 lines. This file, and the SHELL.TBL files are from S.Furihata, Nucl.Inst Meth. in Phys.Res. B171 (2000) 251-258. This file contains mass excesses for 9796 nuclei; they are extracted from the Audi-Wapstra mass table where known (G.Audi and A.H. Wapstra,Nucl.Phys.A 595 (1995) 409-480), supplemented with theoretical values otherwise(P. Moller, J.R.Nix,W.D.Myers, and W.J. Swiatecki, Atomic and Nuclear Data Tables 59 (1995) 185-381, and P.E. Haustein,ibid 39 (1988) 185-393).These data were used with the SHELL.TBL data to generate fission barriers and Q VALUES.

SHELL.TBL (FILE 32)9107 lines.These are shell correction data to extract fission barriers from the experimental or theoretical ground state masses vs. liquid drop saddle point masses from Myers and Swiatecki. These are used internally in the FISGEM fission routine to calculate kinetic energies of fission fragments, while we use a different source for barriers in the Bohr-Wheeler fission calculation.This will be summarized shortly.

PMTABLE (FILE 35)8979 lines. This is a recent mass table due to P.Moller. It can be used to replace MASS.TBL and SHELL.TBL.It was used to get beta2 deformations for GDR calculations.At present it is not in use.

ABUND (FILE 46)287 lines. This is the table of abundances of naturally occuring

isotopes.It is used if the option is selected to use a target of natural isotopic abundances rather than the more usual mono-isotopic target.

Sources of Q values and binding energies for spallation and fission products:

A 1983 Wapstra file is a block data entry in subroutine mass. For nuclides having a mass in this table, that result is used; otherwise a mass excess is calculated internally from the Myers-Swiatecki Lysekil mass formula. The binding energies and Q values are computed from these entries. The OUTPT file lists all the spallation nuclide n,p,alpha binding and pairing energies,and indicates the source as experimental or mass formula.

Level densities:

Generally a Fermi gas form,

$$\rho(E) = E^{-5/4} e^{2(aE)^{0.5}} \tag{1}$$

with a constant T form at low excitation. The constant T is below 0.5 MeV for a Fermi gas, and below (0.5+ 150/A) MeV for the Kataria- Ramamurthy formula.

The level density parameter "a" is generally taken to be slightly greater in calculating the saddle point level density for fission in the Bohr- Wheeler approach (3).We call the parameter af at saddle point, and presently the Alice code,MC uses an arbitrary set of parameters,

$a_f = 1.25 * a; if E > 7.MeV, = 1.22 * A; if E > 14MeV, = 1.18 * a, if E > 21MeV,$
$a_f = 1.15 * a, if E > 28MeV, = 1.10 * a, if E > 36MeV, = 1.08 * a, if E > 42MeV,$
$a_f = 1.06 * a, if E > 48MeV, = 1.04 * a, and above 54.MeV = 1.00 * a.$

This parameterization is found in sub FERMLD; it is based on attempts to reproduce some experimental results, and should be viewed with great caution.Related to this, the theoretical fission barriers which are extracted from the mass formula routine of A. Sierk (LANL,Feb. 1984, private communication 2002) have been modified. In subroutine Seltzer, we fetch the Sierk liquid drop barriers and shell corrections for sub actinide targets of Z¿20. We then reduce the shell correction by 30% in calculating the fission barriers.Thus the barrier calculated in sub. seltzer is given by Bf= B(liquid drop)-shellcorrection*0.7. This effectively reduces the liquid drop barriers. The parameterizations just described for treating fission probably could use some refinement. This should be done using non-zero rotational energies for nuclides.

4. Calculation of angular momenta and isomer yields.

In general, angular momentum information is not part of a Weisskopf- Ewing calculation. However in our MC calculation we may look to the distribution of entrance channel angular momenta from the optical model used to get the reaction cross section, or deduced assuming a classical sharp cutoff model if a cross section is supplied. We then aportion the number of MC events to these spin values according to the partial reaction cross sections at each angular momentum. Thus if we have "N" MC events selected, and

an incident wave of 'l h-bar' with transmission coefficient t_l , the number of events run will be

$$N(l) = N[(2l+1)t_l \pi \bar{\lambda}/(total reaction cross section) \quad (2)$$

where 'lambda-bar is the rationalized wavelength. A minimum N(l) of 1 is established internally, so if one asks for only 1 MC event, more will be calculated due to rounding each partial wave to 1.

The target nucleus may have non-zero spin. If so, the code will automatically determine this from the phtlib file. This spin will be coupled with the entrance channel spin, such that each possible resultant angular momentum 'J' occurs with a weighting proportional to 2J+1. This is done on an event by event basis, so that all couplings are sampled when large 'N' is selected.

The partial wave 'l' implies a radius of interaction, since l=pXR , where p is the projectile channel momentum and R is the radius. We next calculate the energy e and anglesθ,ϕ of each emitted particle. We make the arbitrary assumption that all emissions take place from the initial contact radius R, and calculate the angular momentum change due to the emission as RX(p') , where (p') is the ejectile momentum. This is calculated for the beam direction as: delj=spin vector*cos(θ)*(outgoing momentum)/incident mom.)

Additionally, we calculate an angular momentum projection perpendicular to the beam direction: delprp=delj*sin(θ)$sin(\phi)/cos(\theta)$.

After each ejectile emission, the spin vectors ' spinr' and 'spinperp' are decremented by the respective values for the ejectile. This is done for the precompound cascade, at the end of which the two vectors are combined in quadrature to get a final spin, again designated ' spinr'.

In the evaporation phase, no radius is defined, so a different procedure must be followed to change the angular momentum with successive emissions of neutrons,protons, and alphas. Here we begin by calculating the average angular momentum of each ejectile vs. energy,$l_{ave}(e,\nu)$where 'e' is the energy and$\nu$the particle type. When the nuclear optical model is chosen to calculate inverse reaction cross sections (option INVER=0), the calculation of$a l - ave(e,\nu)$ is obvious; when the sharp cutoff algorithm is used, the values are calculated in subroutine crslav.

For each evaporated particle a random emission angle is selected, and the emission energy similarly selected by MC algorithm. The average angular momentum $l_{ave}(e,\nu)$ is multiplied by $cos(\theta)sin(\phi)$. The nuclear level density is calculated at $U + E_{rot}(j+) and at U + E_{rot}(j-)$, where the j+/- represent the initial 'spinr' plus or minus the calculated l projection . The Erot represent the rotational energies at spin J from the Sierk rotating finite range model. The spin is then apportioned to be coupled + or minus proportional to the nuclear level density ratio at the two possible angular momenta, MC selected. This process is repeated (in sub. EVAP) for each emission. This procedure is followed for spallation yields; for fission fragments, spins are divided upwards or downwards with equal probability.

Isomer yields are determined from the arrays of excitation vs. angular mom- enta for those nuclei with insufficient energy for further emission of n,p, or alpha. Then a series of divides are used in subroutines isomers and iso2 to apportion the population according to spin and excitation.If the ground state spin is J1 and the isomer has a larger spin J2 at energy E2, then : all population below E2 is assigned to the ground state. Above E2, all population with spin below (J1+J2)/2 is assigned as well to the ground state, plus half the population at spin (J1+J2). The remainder is assigned to the isomer yield.

If J2¡ J1, : all population below E2 is assigned to the ground state; above E2 all population above (J1+J2)/2 plus half the cross section at (J1+J2)/2 are assigned to the ground state yield, the remainder is assigned to the iso- mer.These follow the general approach of Vandenbosch and Huizenga (5). For algorithms used in other cases and for two isomer nuclei, refer to sub- routines isomers and iso2. Fission isomers are integrated using the same assumptions in subroutine isomersf.

4.1 Fission isomers

The spins of fission fragments are assumed to result from two sources: the angular momenta of the composite nucleus which undergoes fission, and an angular momentum imparted from the fission process to the fragments. These two results are coupled assuming a 2J+1 weighting among possible final spins.

While it seems reasonable to divide the composite nucleus spin between the fragments proportionally to their moments of inertia, at present the spin is divided equally between light and heavy fragments. The intrinsic spins of the fragments are presently assigned based on results deduced for isomer spins from the spontaneous fission of i^{252}Cf (8). We have parameterized those experimental results and assume that the spin, Lfrag imparted from the fission process to a fragment of mass number Afrag at excitation Efrag is :

$$L_{frag} = 0.0352A_{frag} + 0.00070A_{frag}E_{frag} \tag{3}$$

The Lfrag is coupled randomly with the spin from the fissioning nucleus with 2J+1 weighting, where J is the final spin. Spins are calculated and carried as continuous variables- with some integerizing- then are converted before storing to integer or half integer spins according to the odd or even char- acter of the final nucleus. This is done in the sub EVAP for spallation pro- ducts and in EVAP1 for fission fragments. The spin values Lfrag are decreased for fragments near closed nuclear shells:

if abs(N-82) l.e.2, Lfrag = 0.9 Lfrag
if abs(Z-50) l.e.2, " " "
if abs(N-82) l.e.1, " 0.8 "
if abs(Z-50) " " " "
if N=82, " 0.7 "
if Z=50 " " ".

The algorithms used for fission isomer calculation need benchmarking against experimental independent fission yield results, or yields which are convert- ible to independent yields. At that time these algorithms may be changed. There are also questions which might be addressed at the level of theory: should fragments from lighter systems with more deformed saddle points, and shorter saddle to scission distances be treated for intrinsic spin using an algorithm derived for ^{252}Cf ?

5 Fission cross sections

The fission cross sections and probabilities are calculated using the Bohr -Wheeler model (3) with parameters as described earlier. Once the fission probability has been calculated, there are two possibilities for proceeding. The first is to select a 0 to 1 random number, and if it falls within this probability, determine that the event is fission, and continue. This is a good method if the fission cross section is reasonably large, but results in few or no events if fission is of the order of microbarns with a reaction cross section measured in barns. In this case it is more accurate to multiply the reaction cross section by the fission probability for every event, and do the fission yield/ kinematics calculation for each event. In this approach, the unit of cross section to be divided into particle emission channels is reduced by the fission cross section (which has been moved into the fission channel) before storing. This is the approach we have adopted. It increases the running time, but assures accurate treatment of fission equally for large or small fission cross sections. The physics for this is found in the EVAP subroutine, and the routines called therein for fission barrier heights. Deexcitation of fission fragments is done in the sub. EVAP1, and the kinematics on the evaporated particles from fission is in the FIZKINEM routine called from EVAP1. Running times might be reduced by as much as 30% by treating fission differently maintaining the same accuracy on total fission cross sections, but sacrificing accuracy of fragment yield calcul- ations. The subroutine FIZFRAG is in place to do this, should the option be preferred at a future time.

The mass and charge divisions, as well as fission fragment excitations and channel energies come from routines developed and written by Mashnik and Gudima (7), based on the initial work of Atchison,modified first byFurihata and then by Mashnik/Gudima. The authors are very grateful to these authors for generously making these available for use in the Alice code, and for discussion regarding the routines and physics.

6 Additional latent capabilities

Coincidence gating capabilities exist in a commented form. These gates could be set to print single or double differential spectra gated on ejectile identification-n,p,alpha, on angle and solid angle, and on the exclusive multiplicity of emitted particles. These also

could be reactivated as options.

The deterministic option will likely be reactivated as an option. This gives much faster calculations with similar results for the larger yields. For the Monte-Carlo calculation, we hope to add algorithms for treating deuterons in the entrance channel.

The ENDV output is presently limited to up to 3 particle emission, and only for n,p,4He. The logic being established, it is straightforward to extend the number of exclusive particles treated, as well as the particle types.

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