XXI. MIXR

This module will construct a new PENDF tape with a specified set of reactions that are linear combinations of the cross sections on the input tapes. MIXR can also be used for ENDF tapes, but the input interpolation laws are ignored. The output file contains ENDF File 1 and File 3 sections only, and linear-linear interpolation is assumed.

MIXR can be used for several purposes. When combined with PLOTR, it can be used to construct mixed cross sections for plotting. One example would be to combine the isotopic cross sections given for ENDF/B-VI evaluations into elemental cross sections for comparison with ENDF/B-V data (see the sample input deck below). Another would be to compute the difference between two versions of a particular reaction; plots that simultaneously show one version of a function and the difference between that version and another are sometimes very revealing. In both cases, the mixed cross section is computed on the union grid of its components, and all details are preserved.

Another use for MIXR would be to prepare a new ENDF material to represent a particular "enriched uranium," having a particular amount of ^{235}U mixed with ^{238}U. This file could then be run through the GROUP flux calculator to generate an accurate pointwise flux for enriched uranium mixed with water, or for pins of enriched uranium in a typical reactor lattice. This computed flux could then be used as the weighting flux for computing the self-shielded cross sections of both ^{235}U and ^{238}U in two subsequent GROUPR runs. This approach handles the interference between resonances in ^{235}U and ^{238}U accurately, including proper treatment of all wide and intermediate resonance effects.

A. User Input

The following input instructions were copied from the comment cards at the beginning of the MIXR source. It is always a good idea to check the cards in the current version of the program for possible changes.

```
C     *  USER INPUT --                                                  *
C     *                                                                 *
C     *  CARD 1  --  UNITS                                              *
C     *     NOUT      OUTPUT UNIT FOR MIXED CROSS SECTIONS              *
C     *     NIN1      FIRST INPUT UNIT (ENDF OR PENDF)                  *
C     *     NIN2      SECOND INPUT UNIT                                 *
C     *      ...       CONTINUE FOR NNIN<=10 INPUT UNITS                *
C     *                                                                 *
C     *  CARD 2  --  REACTION LIST                                      *
C     *      MTN       LIST OF NMT<=20 MT NUMBERS FOR                   *
```

```
C     *                   THE OUTPUT REACTIONS                        *
C     *                                                               *
C     *  CARD 3  --  MATERIAL LIST                                    *
C     *     MATN,     LIST OF NMAT<=10 PAIRS (MATN,WTN) OF MAT        *
C     *      WTN       NUMBERS AND ASSOCIATED WEIGHT FACTORS          *
C     *                                                               *
C     *  CARD 4  --  TEMPERATURE                                      *
C     *     TEMP      TEMPERATURE (USE ZERO EXCEPT FOR PENDF TAPES)   *
C     *                                                               *
C     *  CARD 5  --  OUTPUT MATERIAL                                  *
C     *     MATD      MATERIAL NUMBER                                 *
C     *     ZA        ZA VALUE                                        *
C     *     AWR       AWR VALUE                                       *
C     *                                                               *
C     *  CARD 6  --  FILE 1 COMMENT CARD                              *
C     *     DES      DESCRIPTION (60 CHAR MAX)                        *
C     *                                                               *
C     *****************************************************************
```

CARD 1. This card gives the unit numbers for the output that will contain the mixed cross sections and the input files that contain the materials to be mixed together. Note that there is a limit of 10 input materials.

CARD 2. The code currently allows up to 20 mixed reactions to be generated. This card contains a list of the MT numbers for these reactions. The number of reactions is counted automatically.

CARD 3. This card (it may continue onto several lines) contains the MAT numbers and weights for the materials to be mixed. The first pair `MATN`, `WTN` refers to the data on input file `NIN1`; the next pair is for `NIN2`, etc.

CARD 4. The same temperature is used for all of the materials, and its value is given on this card in Kelvin. The appropriate value for ENDF tapes is zero. The temperatures used for PENDF cases must be in the set included on the PENDF tape.

CARD 5. This card gives some values that are needed to construct the ENDF or PENDF file for the output material. `MATD` is the conventional material number. `ZA` is $1000 * Z + A$, where Z is the charge number and A is the atomic mass number for the mixture. Finally, `AWR` is the mass ratio to the neutron for the mixture.

CARD 6. This card contains one line of text to be used for the Hollerith descriptive information in MF=1/MT=451 on the new ENDF tape for the fixture. The final tape on `NOUT` will contain the section MF=1/MT=451 and sections MF=3/MT=MT$_n$ only.

The following sample input deck combines the four isotopes of iron to generate plots for the total cross section (MT=1), the energy-balance heating cross section (MT=301), and the radiation damage cross section (MT=444). See the PLOTR chapter for more information on the part of the input deck that produces the actual graphs.

```
CFS GET XNJOY:/NJOY/91/XNJOYNR
CFS GET TAPE21:/PENDF/5/FE/NATR2
CFS GET TAPE22:/PENDF/6/FE/54
CFS GET TAPE23:/PENDF/6/FE/56
CFS GET TAPE24:/PENDF/6/FE/57
CFS GET TAPE25:/PENDF/6/FE/58
CAT>INPUT <<EOF
 0
 6
 MIXR
 20 -22 -23 -24 -25/
 1 301 444/
 2625 .0590
 2631 .9172
 2634 .0210
 2637 .0028/
 300/
 2600 26000 56.
 *FE-NAT FOR ENDF/B-VI FROM MIXR*/
 PLOTR
 /
 1/
 *ENDF/B-VI IRON*/
 *TOTAL*/
 1 0 2 1 13E6 9./
 0 20E6 2E6/
 /
 0 10 2/
 /
 6 20 2600 3 1 300/
 /
 *ENDF/B-VI*/
 2/
 5 -21 1326 3 1 300/
 0 0 4/
 *ENDF/B-V*/
 1/
 *ENDF/B-VI IRON*/
 *TOTAL*/
 4 0 2 1/
 1E2 1E5/
 /
 /
 /
 6 20 2600 3 1 300/
 /
```

```
 *ENDF/B-VI*/
 2/
 5 -21 1326 3 1 300/
 0 0 4/
 *ENDF/B-V*/
 1/
 *ENDF/B-VI IRON*/
 *HEATING CHECK*/
 1 0 2 1 1E6 2.7E6/
 0 20E6 2E6/
 /
 0 3E6 .5E6/
 *H<EATING (E>V<-BARNS>)*/
 6 20 2600 3 301 300/
 /
 *ENDF/B-VI*/
 3/
 5 -21 1326 3 301 300/
 0 0 4/
 *ENDF/B-V*/
 1/
 *ENDF/B-VI IRON*/
 *DAMAGE CHECK*/
 1 0 2 1 13E6 7E4/
 0 20E6 2E6/
 /
 0 35E4 5E4/
 *D<AMAGE (E>V<-BARNS>)*/
 6 20 2600 3 444 300/
 /
 *ENDF/B-VI*/
 3/
 5 -21 1326 3 444 300/
 0 0 4/
 *ENDF/B-V*/
 99/
 STOP
EOF
XNJOY<INPUT
CFS STORE PLOT:/PENDF/6/FE/NATPLOT
```

The first few lines retrieve the NJOY executable, the ENDF/B-V version of Fe-nat, and the four iron isotopes for ENDF/B-VI. A c-shell "here file" is then created with the input for MIXR and PLOTR. The lines after the `EOF` line take care of executing NJOY and saving the plot file for future use.

Returning to the actual NJOY input cards, note that the MIXR output will be on `TAPE20` in ASCII mode, and the four isotopic input files (in binary mode) will be on `TAPE22` through `TAPE25`. The next input card lists the three reaction types to be written onto the output file; it is followed by four cards giving the isotope

MAT numbers and the atomic fractions that they are to have in the mixture. These mix-specification cards are then followed by a card asking for a temperature of 300 K.

The last two cards in the MIXR section specify the ENDF parameters for the mixed material that will be written on TAPE20. The MAT number is to be 2600 (the standard ENDF-6 value for natural iron), the ZA value is to be 26000, and the AWR value is to be 56.0000 (a rather crude choice). The text line shown will appear in MF=1/MT=451 on the output tape.

At this point, the MIXR module will run and produce its output file. The rest of the input deck reads in this output file and makes a graphical comparison of the mixed elemental cross section with the corresponding elemental values from ENDF/B-V.

B. Coding Details

The heart of MIXR is subroutine GETY. It is similar to GETY1 in NJOY, except that it works with several TAB1 records in parallel. The routine is initialized for up to 10 input TAB1 records on up to 10 input tapes by calling it with X=0 for each tape. It returns the value of XNEXT for each tabulation. The calling program can compare these XNEXT values to determine the lowest energy point for the mixed reaction (the threshold).

On subsequent calls with X>0, MIXR returns the value of Y corresponding to X for the specified tabulation, and it also computes XNEXT for this tabulation. The calling program can loop through all the input tapes, compute the mixed value of Y as a linear combination of the separate GETY results, and compute the next energy grid point as the lowest of the values of XNEXT returned by the separate GETY calls. In this way, the mixed results are obtained on a unionized grid, and no features are lost.

To do its job, GETY has to keep tables of the current location and related parameters on each of the input tapes. These tables will be found in common /GETYC/ with dimension 10.

C. Error Messages

ERROR IN MIXR***MAT AND TEMP NOT FOUND

There is an inconsistency between the requested MATN and TEMP values and the materials found on the input files NIN1, NIN2, ...

`MESSAGE FROM MIXR***MT=xxx NOT PRESENT FOR MAT=xxxx`

This message is just information. If the user asked for construction of, for example, an (n,2n) reaction for an element, and if one of the isotopes did not have an (n,2n) reaction, this message would be issued.

`ERROR IN GETY***NOT PROPERLY INITIALIZED`

The subroutine `GETY` has to be called with `X=0` for each material/section combination to be introduced into the mixed reaction before it is called with `X>0`.

CONTENTS