25 GASPR

The GASPR module will add gas production reactions (MT=203-207) to the PENDF file. Any existing gas-production sections on the input PENDF file are removed, and the file directory is updated to show the new reactions. This module can be run anywhere in the PENDF preparation sequence, but as a practical matter is should follow BROADR.

This chapter describes the GASPR module in NJOY2016.0.

25.1 Gas Production

The light products of nuclear reactions – namely, protons, deuterons, tritons, ^{3}He's, and alphas – can accumulate as gases in a nuclear system. The resulting hydrogen, deuterium, tritium, ^{3}He, and ^{4}He buildup can have important effects on the original material, such as causing embrittlement. In other cases, the gas may even be the desired product, such as in tritium production.

Keeping track of the total production of each gas species is complicated. Gases can sometimes be determined from the MT number for the reaction; for example, an (n,α) reaction produces one ^{4}He per reaction. The gas might be a residual nucleus as in ^{2}H(n,2n)^{1}H or ^{9}Be(n,2n)2α. Sometimes, the ENDF LR flags are used to indicate that the residual nucleus from a reaction breaks up by further particle emission. An example of this is ^{16}O(n,n$_6$)α represented using MT=56/LR=22. In other cases, the yield per reaction for the light product may be tabulated directly (and even be fractional) when File 6 is used for the reaction. This is common for the high-energy data (150 MeV) introduced for ENDF/B-VI Release 6. GASPR goes through all the reactions in the evaluation and adds up all these various contributions to get the net production of each of the light species.

The ENDF format assigns the MT values from 203 to 207 to represent the production of hydrogen, deuterium, tritium, ^{3}He, and ^{4}He, but only a few evaluators have supplied these data in the past. By using GASPR to generate these data at the PENDF stage, a number of possible inconsistencies are avoided. Therefore, when gas-production MT values are found, GASPR removes them in favor of the ones that it calculates.

When the code runs, it prints out a summary of which reactions contribute to the production of each gas. Here is an example for aluminum from ENDF/B-VII.0:

```
mf6,mt5 found

the gas production threshold is  1.8969E+06 ev

found  1038 points

pendf mt  mt203  mt204  mt205  mt206  mt207
--------  -----  -----  -----  -----  -----
       5    ***    ***    ***    0.0    ***
      22    0.0    0.0    0.0    0.0    1.0
      28    1.0    0.0    0.0    0.0    0.0
      32    0.0    1.0    0.0    0.0    0.0
      33    0.0    0.0    1.0    0.0    0.0
      45    1.0    0.0    0.0    0.0    1.0
     103    1.0    0.0    0.0    0.0    0.0
     104    0.0    1.0    0.0    0.0    0.0
     105    0.0    0.0    1.0    0.0    0.0
     107    0.0    0.0    0.0    0.0    1.0
     108    0.0    0.0    0.0    0.0    2.0
     111    2.0    0.0    0.0    0.0    0.0
     112    1.0    0.0    0.0    0.0    1.0
     117    0.0    1.0    0.0    0.0    1.0

*** means that the yield is energy dependent

found 8 temperatures
```

25.2 User Input

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

Users are cautioned that only tape numbers are input. GASPR assumes that the first material read from each tape is the material to be processed. Therefore, if dealing with multi-material tapes MODER should be run to create a single material tape for input to GASPR.

```
! card 1
!    nendf    unit for endf tape
!    nin      unit for input pendf tape
!    nout     unit for output pendf tape
```

25.3 Coding Details

Subroutine `gaspr` is exported by module `gaspm`. The code first checks the directory in File 1 of the ENDF tape to see whether MF=6/MT=5 is present (see `mf6mt5`). If so, it reads through the MT=5 section of File 6 and saves the various light-particle yields in the array `six` using a set of pointers like `l203`, `l204`, and so on.

GASPR then proceeds to read through the input PENDF tape. It copies all the sections up to point where the gas production sections will be inserted to a scratch file. It then goes through all these reactions computing the direct products and the residual nucleus (with full account of the LR flags) and determines the lowest threshold for gas production. It then goes back through the scratch file again to get the energy grid for the total cross section starting at the threshold (see `egas`). It continues looping over all the reactions on the file, determining again what the direct products and residual nuclei are, and accumulating the gas production values in the array `sgas(particle,energy)`.

When all the reactions have been processed, GASPR goes back and updates the directory in MF=1/MT=451 to reflect the new reactions that have been added. It copies all the reactions on the scratch file to the output PENDF tape. It constructs new MF=3 sections for each of the gas-production reactions that was found. And then it copies the remainder of the input PENDF tape to the output file.

25.4 Error Messages

`error in gaspr***npend and noutp must both be ...`
: The mode of the PENDF tape must not change, because many of the sections are simply copied.

`error in gaspr***too many gas production energy points.`
: Should not occur, `maxg` used to allocate space for `egas(maxg)` and `sgas(5,maxg)` is determined from the input file.