**Updating NJOY2016.72 for FENDL, IRDFF, ADS-Lib, and WIMSD library processing.**

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**Introduction**

The IAEA Nuclear Data Section (IAEA/NDS) maintains a set of nuclear data libraries for applications like FENDL, IRDFF, ADS-Lib and WIMSD libraries. These libraries were processed by different versions of the NJOY code system. They required a set of NJOY updates for a correct processing. Most of the updates have been included in the NJOY2016.71, but still some important updates are missing, and recent updates are also needed for processing latest released evaluated nuclear data libraries. The new updated version NJOY2016.71+ can successfully process all the IAEA/NDS application libraries mentioned above. Some of the updates are also important for processing others evaluated nuclear data libraries. This report summarizes the implementation of the required updates.

**Updating NJOY2016.72 for processing IAEA/NDS libraries**

A total amount of twenty-four modules were updated. A brief description of the main updates is given below by module in alphabetical order:

Module acecm

* A set of updates is related to the introduction of extended MT numbers for dosimetry and photonuclear production data, particularly if acer is used to check an ACE-formatted file created by other code. This issue is important for dosimetry data from MT5.
* Modification of *subroutine mtname* for charged particles. Correction of some reaction names.
* The Fortran integer format descriptor i6 is changed to i9 in *subroutine advance\_to\_locator* considering the size of array xss (more than ten million of elements)

Module acedo

* A set of updates was included to allow the usage and printout of extended MT numbers.

Module acefc

* Starting from the Japanese updates [1, 2] for processing incident charged particle evaluations from JENDL-5 a new input option was implemented for controlling whether the endf/mf6/law7 is converted to endf/mf6/law1 or not when the new format option is invoked (newfor=1). It is important for charged particle transport simulations using MCNP-6.1 and MCNP-6.2 where the law61 is not working. A full implementation of this option was introduced in the NJOY version NJOY2016.71. Updates applied to several *subroutines* like *acetop, acelf6, topfil , acelod,* and *acelcp*.
* Checking of law67 was added in the *subroutine consis*
* Corrections to consider incident charged particles (awi≠1) in subroutines *consis* and *topfil*
* The *subroutine unionx* was patched to correctly include extra points for large intervals in the unionized grid for charge particles. Current implementation can skip the point before the last and never densify the last interval. It is important for high energy evaluations.
* The *subroutine unionx* was also patched to consider the values supplied on the section MF3/MT2 for the elastic scattering of charged particles.
* The *subroutine acelod* was corrected to manage the event when only the elastic scattering produces the incident particle (mtnr=0). It is the case of B-10 from FENDL-32 proton evaluated nuclear data. It can affect the calculation of the elastic cross section for charged particles, because the scattering data required by *subroutine acecpe* is not loaded into xss array.
* Patching *subroutine acelod* to consider the case that the reaction MT5 does not produce the incident particle but produces others particles. It is the case for example of 1-H-2 for incident protons from JENDL-5. The logic for including producing and not- producing incident particle reactions was updated.
* Warning when LAB reference system is used in MF6/LAW6. NJOY2016 can not treat MF6/LAW6 in the LAB system. CM system is enforced. Additionally, the generation of the normalized energy distribution for MF6/LAW6 was reorganized.
* The values of ZA for incident and product particles were corrected in the call of *subroutine bachaa* for charged particles.
* Correction to the smoothing option (ismooth=1) for histograms when the first secondary energy is not 0.0 or 0.00001 eV. It is important for some FENDL evaluations coming from TENDL-2011.
* *Subroutine acecpe* was modified to avoid singularities and to correctly consider all the mf6/mt2/law=5 representations
* Correction of a typo and patching the subroutine acelf6 when tabulated data (mf6/law1/lang2) is converted to Kalbach formalism (mf6/law1/lang2) for newfor=0.
* Patching *subroutine acelcp*, because for several energy distribution, including law67, the energy distribution array was wrong. The arrays describing the probability of law were missed or incorrectly loaded into xss array.
* Patching *subroutine acelpp* for preparing the unified grid part of a law1 for discrete photons.
* Modification of *subroutines aplodd* and *aploxp* for plotting law67. Correction of recoil heat plotting.
* Minor correction for recoil heat plotting and increasing arrays sizes for large evaluations.

Module acepa

* Increased dimension of main array

Module acepn

* Treatment of Kalbach formalism when na=2.
* Generalization of coding for some cases where more than one interpolation law (nr>1) is applied.

Module acer

* Modification to consider the new input parameter no7 for converting endf/mf6/law7 to ace/law67 when newfor=1. Useful for charged particle processing.

Module broadr

* Minor change to keep some legacy options to avoid problems with some Fortran compilers.

Module endf

* Rewind the tape before use it in subroutine tpidio. Needed when running multiple modules in sequence.

Module errorr

* A checking and corrective action was introduced if a negative variance is found. Warning is printed.

Module gaspr

* Included direct production of two alpha particles from Li-8 residual (Li-8->Be-8->2α)
* Minor changes to process reaction with MT>200 from JENDL-5

Module groupr

* Minor code reordering and increasing the size of some arrays.

Module heatr

* Implementation of the kinematic method for estimating the total and partial KERMA factors. Adapted from the corresponding Japanese original patches by Kazuaki Kosako and Chikara Konno. Despite recent improvements, heating numbers can be wrong in some evaluations. The option to replace the calculated values by the upper kinematic limit is still relevant.
* Implementation of corrections described in reference [3] to patch the heating and damage calculation for MT102.

Module leapr

* Minor code changes reported by leapr users.

Module locale

* Updated variables *lab* and *mx* according to this version

Module main

* Updated comments according to this version (NJOY2016.71+)

Module mainio

* Changed to use the legacy options to avoid problems with some Fortran compilers.

Module matxsr

* Corrected a Fortran format descriptor that produce wrong data when ASCII matxs-formatted files are produced. The group energy boundaries can be corrupted. Important for FENDL processing.

Module plotr

* Increase some arrays dimension for large plots. Consistency with module viewr dimensions is required.

Module purr

* Implemented a procedure for managing exceedingly small total cross section samples. It was important for processing La-139 from FENDL-3.1 [4, 5].

Module reconr

* Implemented the correct treatment of the elastic scattering cross section for charged particles. For mf6/law5/ltp≥12, the mf3/mt2 section should contain the values of the “nuclear plus interference” cross section σNI, which can be negative. For ltp=1 or ltp=2, the values should be 1.0 even at the threshold energy. Otherwise, the elastic scattering cross section could be incorrectly calculated in *subroutine acecpe*.

Module util

* Close the scratch tape before opening it in *subroutine openz*, if needed
* Minor correction in *function sigfig* [1]

Module vers

Updated variables *vers* and *vday* according to this version.

Module viewr

* Increase some arrays dimension for large plots. Consistency with module plotr dimensions is required.

Module wimsr

* Correction for wimsd5 formatted library (iverw=5)

The size of some arrays was increased in the previously listed modules for future release of large evaluations.

The rest of NJOY modules are taken as they are in NJOY2016.71.

The more important updates are those applied to reconr, heatr, purr, acecm, acer, acefc acedo, matxsr, and wimsr.

**References**

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2. Modification of NJOY2016.67 for JENDL-5 photonuclear sublibrary, <http://rpg.go.jp/download/ace_lib/acej50/20221205/NJOY2016.67.modification.r2.pdf>
3. Wen Yin, Tiejun Zu, Liangzhi Cao, Hongchun Wu, “Remarks and improvements on neutron KERMA factors and radiation damage cross sections calculated by NECP-Atlas and NJOY21 using different evaluated nuclear data libraries”, Annals of Nuclear Energy 164 (2021) 108624
4. Chikara Konno, Kenichi Tada, Saerom Kwon, “MATXS multigroup file problem due to NJOY unresolved resonance processing”, ICRS14/RPSD2020, 2020
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