

Modification of NJOY2016.65 for
JENDL-5 neutron, photoatomic, and charged particle sublibraries (Rev.2)

It is necessary to modify NJOY2016.65 in order to process JENDL-5 neutron, photoatomic, and charged particle sublibraries. Here we show the modifications of NJOY2016.65. Note that only the heart module in NJOY2016.65 were used for JENDL-5 neutron sublibrary because FRENDY was mainly used. You must use the modifications with your own responsibility.

1. Modification for JENDL-5 neutron sublibrary (1)

We encountered the following errors.

error in endf illegal TAB1, nbt(nr)/=np for mf/mt = 3/ 1 in acer processing of Ni58 etc.

error in topfilnxc.gt.nxcmax. in acer processing of Cu63 etc.

Abort trap: 6 in purr processing of Gd155 etc.

Our solutions for the errors are as follows.

(1) acefc.f90

line 27

```
integer,parameter::nxcmax=500  
--> integer,parameter::nxcmax=1000
```

line 1940

```
integer::nep,ll,iep,nb,nw,iend,nwmax,nin0,latng,i,np  
--> integer::nep,ll,iep,nb,nw,iend,nwmax,nin0,lang,i,np,nw2
```

line 2314

```
call tab2io(nin,0,0,b,nb,nw)  
--> call tab2io(nin,0,0,b,nb,nw2)
```

line 2337

```
call tab2io(0,nout,0,b,nb,nw)  
--> call tab2io(0,nout,0,b,nb,nw2)
```

~~line 3892~~

~~nncd=50~~

~~--> nmed=100~~

(2) purr.f90

line 1101

nthr=140

--> nthr=500

2. Modification for JENDL-5 neutron sublibrary (2)

We encountered negative heating numbers due to energy balance problem. We replaced heating numbers from the energy balance method with those from the kinematics method by modifying heart.f90 and setting the new input parameter kerma to 1. We also modified heart.f90 based on Chinese researchers' studies (Wen Yin, et al., Annals of Nuclear Energy 164 (2021) 108624, Shengli Chen, Nuclear Instruments and Methods in Physics Research B 513 (2022) 1–8).

(1) heatr.f90

line 37

real(kr)::emc2,tm,rtm

--> real(kr)::emc2,tm,rtm

integer::kerma

line 98

! (default from built-in table)

--> ! (default from built-in table)

! kerma 0/1=energy balance kerma/kinematics kerma

! (default=0)

line 164

read(nsysi,*) matd,npk,nqa,ntemp,local,iprint,break

--> kerma=0

read(nsysi,*) matd,npk,nqa,ntemp,local,iprint,break,kerma

line 217

do i=1,npk

if (mtk(i).eq.443.and.kchk.eq.0) kchk=2

if (mtk(i).eq.301) isave=i

enddo

--> do i=1,npk

if (mtk(i).eq.443.and.kchk.eq.0) kchk=2

```
    if (mtk(i).eq.301) isave=i
  enddo
  do i=1,npk
    if (mtk(i).eq.443) go to 100
  enddo
  if (kerma.eq.1) call error('heatr',&
    ' no mt=443 in input!', ' ')
100 continue
```

line 262

```
  endif
  if (ntemp.eq.0) ntemp=100
--> endif
  write(nsyso,('&
    &" kerma (0 e-balance, 1 kinematics) .... ",i10)')&
  kerma
  if (ntemp.eq.0) ntemp=100
```

line 2944

```
  if (irec.gt.0) pe=1
--> if ((mth.ne.102).and.(irec.gt.0)) pe=1
```

line 3228

```
  xx=c(l)
--> xx=abs(c(l))
```

line 5681

```
  integer,parameter::nwscr=10000
--> integer,parameter::nwscr=10000
  integer::mt302,mt318,mt402,mt443
```

line 5702

```
  do i=2,npk
    if (mtp(i).ge.442) then
      npkd=npkd-1
      npktd=npktd-1
    endif
  enddo
--> do i=2,npk
```

```

    if (mtp(i).ge.442) then
      npkd=npkd-1
      npktd=npktd-1
    endif
  enddo
  mt443=0
  mt318=0
  mt402=0
  mt443=0
  if (kerma.eq.1) then
    do i=2,npk
      if (mtp(i).eq.302) mt302=(npk-1)*2+i
      if (mtp(i).eq.318) mt318=(npk-1)*2+i
      if (mtp(i).eq.402) mt402=(npk-1)*2+i
      if (mtp(i).eq.443) mt443=i
    enddo
  endif

```

line 5784

```

  118 continue
    i=i+2
    scr(ibase+i-1)=c(1)
    scr(ibase+i)=c(inpk)
--> 118 continue
    i=i+2
    scr(ibase+i-1)=c(1)
    scr(ibase+i)=c(inpk)
    if (kerma.eq.1) then
      if (mth.eq.301) scr(ibase+i)=c(mt443)
      if (mth.eq.302) scr(ibase+i)=c(mt302)
      if (mth.eq.318) scr(ibase+i)=c(mt318)
      if (mth.eq.402) scr(ibase+i)=c(mt402)
    endif

```

line 5815

```

    call afend(0,nscr)
    call repoz(nscr)
--> call afend(0,nscr)
    call repoz(nscr)

```

```

if (mt443.ne.0) then
  write(strng,('mt=301 is replaced with mt=443! '))
  call mess('heatr',strng,' ')
endif
if (mt302.ne.0) then
  write(strng,('mt=302 is replaced with kinematics one! '))
  call mess('heatr',strng,' ')
endif
if (mt318.ne.0) then
  write(strng,('mt=318 is replaced with kinematics one! '))
  call mess('heatr',strng,' ')
endif
if (mt402.ne.0) then
  write(strng,('mt=402 is replaced with kinematics one! '))
  call mess('heatr',strng,' ')
endif

```

3. Modification for JENDL-5 photoatomic sublibrary

We encountered the following errors.

fortrtl: severe (408): fort: (2): Subscript #1 of the array XSS has value 999001 which is greater than the upper bound of 999000 in acer processing of N.

fortrtl: error (140): floating inexact in acer processing of Mg etc.

The first error occurred because the same energy exists in the ENDF-6 file. We fixed this error by modifying util.f90 as follows

(1) util.f90

line 377

```

if (x.ne.zero) then
  aa=log10(abs(x))
  ipwr=int(aa)
  if (aa.lt.zero) ipwr=ipwr-1
  ipwr=ndig-1-ipwr
  ii=nint(x*ten**ipwr+ten**(ndig-11))
  if (ii.ge.10**ndig) then
    ii=ii/10
    ipwr=ipwr-1
  endif

```

```

        ii=ii+idig
        xx=ii*ten**(-ipwr)
    endif
--> if (x.ne.zero) then
        aa=log10(abs(x))
        ipwr=int(aa)
        if ((ndig.eq.9).and.(aa.gt.zero).and.(aa-ipwr.lt.1.0e-6_kr)) ipwr=ipwr-1
        if (aa.lt.zero) ipwr=ipwr-1
        ipwr=ndig-1-ipwr
        ii=nint(x*ten**ipwr+ten**(ndig-11))
        if (ii.gt.10**ndig) then
            ii=ii/10
            ipwr=ipwr-1
        endif
        ii=ii+idig
        xx=ii*ten**(-ipwr)
    endif

```

The second error occurred because NJOY2016.65 requires atomic relaxation data, which were not required in the old NJOY codes. We used JENDL-5 atomic relaxation sublibrary in this processing.

4. Modification for JENDL-5 charged particle sublibraries

NJOY2016.65 produces ACE files of LAW=61 for JENDL-5 charged particle sublibraries, where LAW=7 is adopted. Unfortunately MCNP6.2 and PHITS3.27 cannot treat charged particle ACE files of LAW=61 correctly, while they can do charged particle ACE files of LAW=67. NJOY2016.65 has a hidden function to produce charged particle ACE files of LAW=67, but the function is not perfect. We completed the hidden function as follows and produced charged particle ACE files of LAW=67. We also changed the interpolation of 22 to 2 in file6 mt=5 to 2 for the Be9 proton ACE file because MCNP6.2 and PHITS3.27 do not support the interpolation of 22.

(1) acer.f90

line 158

```

!           NOTE: ismooth=0 is the default value in njoy99.
--> !           NOTE: ismooth=0 is the default value in njoy99.
!   no7   convert law=7 sections to law=61 or law=67
!           (0=law67, 1=law61, default=1)

```

line 240

```
integer::newfor,iopp,ismooth  
--> integer::newfor,iopp,ismooth,no7
```

line 313

```
ismooth=1  
read(nsysi,*) newfor,iopp,ismooth  
write(nsyso,'(&  
  &" new formats ..... ",i10/&  
  &" photon option ..... ",i10/&  
  &" smoothing option ..... ",i10))&  
  newfor,iopp,ismooth  
--> ismooth=1  
  no7=0  
  read(nsysi,*) newfor,iopp,ismooth,no7  
  write(nsyso,'(&  
    &" new formats ..... ",i10/&  
    &" photon option ..... ",i10/&  
    &" smoothing option ..... ",i10/&  
    &" law7 option ..... ",i10))&  
    newfor,iopp,ismooth,no7
```

line 440

```
hk,izn,awn,matd,tempd,newfor,iopp,ismooth,thin)  
--> hk,izn,awn,matd,tempd,newfor,iopp,ismooth,no7,thin)
```

(2) acefc.f90

line 90

```
subroutine acetop(nendf,npend,ngend,nace,ndir,iprint,itpe,mcnp,&  
  suff,hk,izn,awn,matd,tempd,newfor,iopp,ismooth,thin)  
--> subroutine acetop(nendf,npend,ngend,nace,ndir,iprint,itpe,mcnp,&  
  suff,hk,izn,awn,matd,tempd,newfor,iopp,ismooth,no7,thin)
```

line 99

```
integer::nendf,npend,ngend,nace,ndir,iprint,itpe,matd,newfor,iopp,ismooth,i  
--> integer::nendf,npend,ngend,nace,ndir,iprint,itpe,matd,newfor,  
iopp,ismooth,no7,i
```

line 198

```
call topfil(nendf,mscr,matd,newfor)
--> call topfil(nendf,mscr,matd,newfor,no7)
```

line 1919

```
subroutine topfil(nin,nout,matd,newfor)
--> subroutine topfil(nin,nout,matd,newfor,no7)
```

line 1954

```
!--this flag says convert law=7 to law=1
integer::no7=1
--> !--this flag says convert law=7 to law=67 or law=61
integer::no7
```

line 2474

```
l=l+66
--> l=l+300
```

line 5796

```
law=l2h
--> law=l2h
ll=1+nw
do while (nb.ne.0)
  call moreio(nin,0,0,scr(ll),nb,nw)
  ll=ll+nw
enddo
```

line 5850

```
call acecpe(next,scr,nin,awr,awp,&
  spi,ne,lidp,ie,il,nes)
--> if (mth.eq.2) then
  call acecpe(next,scr,nin,awr,awp,&
    spi,ne,lidp,ie,il,nes)
else
  call acensd(ir,next,scr,nin,ltt3,lttn,&
    ltt,last,law,ne,ie,il,iso,newfor)
endif
```

line 6288


```
real(kr),parameter::rmin=1.e-30_kr
--> real(kr),parameter::rmin=1.e-30_kr
    real(kr),parameter::zero=0
```

line 6299

```
call tab1io(nin,0,0,scr,nb,nw)
--> call tab1io(nin,0,0,scr,nb,nw)
    ll=1+nw
    do while (nb.ne.0)
        call moreio(nin,0,0,scr(ll),nb,nw)
        ll=ll+nw
    enddo
```

line 6342

```
iint=nint(scr(8))
--> iint=nint(scr(8))
    if (iint.eq.22) iint=2
```

line 6365

```
renorm=1/xss(next+3*n)
--> renorm=1.0
    if (xss(next+3*n).ne.zero) renorm=1/xss(next+3*n)
```

line 7763

```
intmu=l1h
--> intmu=scr(jscr+7)
```

line 7777

```
intep=nint(scr(jscr+7))
--> intep=nint(scr(jscr+7))
    if (intep.gt.2) intep=2
```

line 7803

```
renorm=1/xss(nexd+3*npep)
--> renorm=1.0
    if (xss(nexd+3*npep).ne.zero) renorm=1/xss(nexd+3*npep)
```

~~line 9019~~

```
integer::next,matd,nin
```

→ integer::next,matd,nin,newfor

line 9890

```
intx=nint(scr(lld+7))  
--> intx=nint(scr(lld+7))  
    if (intx.eq.22) intx=2
```

line 9891

```
xss(na+ie)=scr(lld+1)  
--> xss(na+ie)=scr(lld+1)/emev
```

line 10582

```
intmu=l1h  
--> intmu=scr(ll+7)  
    if (intmu.eq.22) intmu=2
```

~~line 10602~~

```
intop=nint(scr(ll+7))  
--> intop=nint(scr(ll+7))  
    if (intop.eq.22) intop=2
```

line 10754

```
do while (mtt.ne.mt)  
    ir=ir+1  
    mtt=nint(xss(mtr+ir-1))  
    k=nint(xss(lsig+ir-1))+sig-1  
    n=nint(xss(k+1))  
    iaa=nint(xss(k))  
    q=xss(lqr+ir-1)  
enddo  
--> do while (mtt.le.mt)  
    ir=ir+1  
    mtt=nint(xss(mtr+ir-1))  
    k=nint(xss(lsig+ir-1))+sig-1  
    n=nint(xss(k+1))  
    iaa=nint(xss(k))  
    q=xss(lqr+ir-1)  
    if (ir.eq.nprod) exit  
enddo
```

line 13814

```
nrr=nint(xss(l))
call write_integer(nout,l)          ! NR
if (nrr.gt.0) then
  call write_integer_list(nout,l,2*nrr) ! NBT, INT (each NR)
endif
ne=nint(xss(l))
call write_integer(nout,l)          ! NE
call write_real_list(nout,l,ne)     ! E (NE values)
ielocator=l
call write_integer_list(nout,l,ne)  ! L (NE values)
do j=1,ne
  call advance_to_locator(nout,l,dlwh+nint(xss(ielocator))-
  call write_integer(nout,l)        ! INTMU
  nmu=nint(xss(l))
  call write_integer(nout,l)        ! NMU
  call write_real_list(nout,l,nmu)  ! MU (NMU values)
  oelocator=l
  call write_integer_list(nout,l,nmu) ! L (NMU values)
  do k=1,nmu
    call advance_to_locator(nout,l,dlwh+
    nint(xss(oelocator))-1)
    call write_integer(nout,l)      ! INTEP
    nep=nint(xss(l))
    call write_integer(nout,l)      ! NPEP
    call write_real_list(nout,l,3*nep) ! Eout, PDF, CDF (each NMU values)
    oelocator=oelocator+1
  enddo
  ielocator=ielocator+1
enddo
--> do j=1,ne
  call write_integer(nout,l)        ! INTMU
  nmu=nint(xss(l))
  call write_integer(nout,l)        ! NMU
  call write_real_list(nout,l,nmu)  ! MU (NMU values)
  oelocator=l
  call write_integer_list(nout,l,nmu) ! L (NMU values)
  do k=1,nmu
```

```
call write_integer(nout,l)      ! INTEP
nep=nint(xss(l))
call write_integer(nout,l)      ! NPEP
call write_real_list(nout,l,3*nep) ! Eout, PDF, CDF (each NMU values)
oelocator=oelocator+1
enddo
enddo
```

~~line 19394~~

```
intmu=nint(a7(loci))
--> intmu=nint(a7(loci))
--- if (intmu.eq.22) intmu=2
```

~~line 19410~~

```
intmu=nint(a7(loci))
--> intmu=nint(a7(loci))
--- if (intmu.eq.22) intmu=2
```

(3) gaspr.f90

line 273

```
if (mth.gt.200.or.mth.eq.0) then
--> if (mth.gt.202.or.mth.eq.0) then
```

line 287

```
if (mth.gt.200.and.mth.lt.mpmin) go to 245
--> if (mth.gt.202.and.mth.lt.mpmin) go to 245
```

line 475

```
if (mth.gt.200.and.mth.lt.mpmin) go to 310
--> if (mth.gt.202.and.mth.lt.mpmin) go to 310
```

line 950

```
if (nint(a(j+3)).eq.3.and.nint(a(j+4)).gt.200) idone=1
--> if (nint(a(j+3)).eq.3.and.nint(a(j+4)).gt.202) idone=1
```

line 1038

```
if (mth.gt.200.or.mth.eq.0) then
--> if (mth.gt.202.or.mth.eq.0) then
```