GRUCON-D 2016: Cross Section Reconstruction by Multilevel-Multichannel Reich-Moor Limited Formulae

Introduction

Main purpose
To remove the identified limitations of GRUCON that will enable a broader application of the code system.
Statement of Work
- Expand the RXTXS module, to reconstruct cross sections from multilevel – multichannel Reich-Moor Limited formula (LMF=7);
- Expand the ACE module, to generate ACE files for all representations of energy-angle distributions from the ENDF MF=6 file;
- Verify the GRUCON/ RXTXS module, by comparing Fe-56 cross sections, generated from the evaluated data file, with PREPRO-2015 calculations;
- Validate the GRUCON/ACE module, by comparing neutron leakage spectra, measured on iron spheres and calculated from ACE files, prepared by GRUCON code.

The usage in the evaluated data libraries the LMF=7 advanced format for resonance parameters representations led to the need of the structural changes of the GRUCON package. The *R* structure has been kept, but completed by additional structure *RM*, adequate for representation of resonance parameters for the multilevel-multichannel Reich-Moor formalisms. The new *RM* structure is described in the Appendix A.

The implementation of the new structure has led to revision of the system and functional components of the package:

- the system subroutine LOADRM assigned to exchange by the *RM* data structure between operative memory and the segments of the direct access files – segments of the internal library of the package (BSP) has been added;
- the subroutine RMLFOR7 has been added to the ENDF input module to read these data form ENDF file and convert to the standard structure *RM*
- the service module SELECT, EXTRA have been adjusted to recognize this data structure;
- the output module TABLE for printing data in the easy readable form has been supplemented by corresponding subroutine TABRM (see example in the Appendix B;
- the functional module RXTXS has been supplemented by subroutines RML2S and RFRML, assigned for reconstruction detailed cross sections from *RM* structure of resonance parameters.

  In the last one (RFRML), the formulas for reconstruction partial cross section from the ENDF manual [1] has been implemented:

$$\sigma_{elastic} = \frac{4\pi}{k_\alpha^2} \sum_{J^\pi} \left[\sin^2 \phi_c (1 - 2X_{cc}^i) - X_{cc}^r \sin(2\phi_c) + \sum_{c'} |X_{cc'}|^2 \right]$$

$$\sigma_{capture} = \frac{4\pi}{k_\alpha^2} \sum_{J^\pi} \sum_{c} g_{J\alpha} \sum_{c} \left[X_{cc}^i - \sum_{c'} |X_{cc'}|^2 \right]$$

$$\sigma_{reaction} = \frac{4\pi}{k_\alpha^2} \sum_{J^\pi} g_{J\alpha} \sum_{c} \left[X_{cc}^i - \sum_{c'} |X_{cc'}|^2 \right]$$

where

$$R_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c} \gamma_{\lambda c'}}{E_\lambda - E - i\Gamma_{\lambda\gamma}/2} + R_c^b \delta_{cc'}$$

$$X_{cc'} = P_c^{1/2} L_c^{-1} \sum_{c''} Y_{cc''}^{-1} R_{c''c'} P_{c'}^{1/2}$$

$$Y_{cc''} = L_c^{-1} \delta_{cc''} - R_{cc''}$$

$$L_c = S_c - B_c + iP_c$$

and *Pc* and *Sc* are penetrability and shift factors, and Bc are boundary constants. Total is calculated as sum of partial cross sections.

2. Verification procedure

Verification of the advanced GRUCON package has been performed on the CIELO evaluation of the Fe-56 through the procedure proposed by Daniel Lopez Aldama, based on usage of capabilities of the PREPRO-2015 preprocessing code system [2]. The GRUCON input, used in the procedure is in the Appendix C. The two set cross section has been compared: for zero and room temperatures, prepared with tolerance parameter eps=0.001. The results are shown in Figures in the Appendix D. It was fond no contradictions between these two sets within declared tolerance, except energy intervals in vicinity of threshold energies. As can be seen on the pictures, in these intervals the cross sections in these intervals are ~1.e-6 barn, so, discrepancy can be considered as unimportant.

3. Expansion of the ACE module

The limitations of data processing capability of the previous version GRUCON in regard to the ACE file preparation task are largely removed by expanding the ACE module on the all representations lows in secondary neutron distributions: *E*, angle ***A*** and energy-angle *AE*. Now the list of the ACE data tables, AND (angular distributions) and DLW (energy and energy angular distributions), that can be prepared by the ACE module of GRUCON, includes the following representation laws:

LAW=1 Tabular Equi-Probable Energy bins

LAW=3 Level Scattering

LAW=4 Continuous Tabular Distribution

LAW=5 General Evaporation Spectrum

LAW=7 Simple Maxwell Fission Spectrum

LAW=9 Evaporation Spectrum

LAW=11 Energy Dependent Watt Spectrum

LAW=12 Tabular Linear Fuctions

LAW=44 Kalbach-87 Formalism

LAW=61 Like 44 but angular distribution instead of Kalbach-87

LAW=66 N-Body Space Distribution

Only one of them - Laboratory Angle–Energy Law (LAW=67) is not yet implemented, due to the evaluation with this representation is not found in the library.

4. ACE library preparation

For integral testing of the new edition of the GRUCON-D, the processing of the EBDF/B-VII.1 general purpose sub-library (424 materials were included) and thermal scattering data sub-library (H_H2O, H_CH2, H_ZrH, D_D2O, Be_met, Be_BeO, C_gph) has been performed. The GRUCON input for preparation of point-wise ACE from ENDF data for fast and thermal neutron is in the Appendix E.

The most of materials (420) has been processed successfully with only warning diagnostics. The problem cases are under consideration.

5. Integral testing of the ACE files.

Two integral testing runs have been performed with aim to check the prepared through GRUCON packages ACE point-wise cross section files:

- k-eff Monte-Carlo calculations,
- leakage spectra Monte-Carlo calculations.

For the first run, the comparison with experimental results for 51 critical assemblies from International Handbook ICSBEP [4] have been performed. The results are in the
Appendix F.

In the second run, 5 Fe shells with 14MeV neutron source, described in the SINBAD radiation shielding data base [5] were used, namely:

- iron shell No. 1 (r= 4.5 cm, wall thickness = 2.5 cm),
- iron shell No. 2 (r=12.0 cm, wall thickness = 7.5 cm),
- iron shell No. 3 (r=12.0 cm, wall thickness =10.0 cm),
- iron shell No. 4 (r=20.0 cm, wall thickness =18.1 cm),
- iron shell No. 5 (r=30.0 cm, wall thickness =28.0 cm)

The ENDF/B-VII.1 evaluated data library has been used for the ACE file preparation. In the leakage spectra calculations, two evaluations of the Fe-56 has been compare with experimental results: ENDF/B-VII.1 and CIELO (see Appendix G).

References

1. https://www.oecd-nea.org/dbdata/data/manual-endf/endf102.pdf
   M. Herman and A. Trkov, CSEWG Document ENDF-102 Report BNL-90365-2009 Rev.1,National Nuclear Data Center Brookhaven National Laboratory, Upton, NY 11973-5000
2. D.E. Cullen, "PREPRO 2015: 2012 ENDF/B Pre-processing Codes", IAEA-NDS-39, Rev. 16 (January 31, 2015)
3. J. S. Hendricks, "MCNP4C2," LANL Memo X-5:RN (U)-JSH-01-01 (30 January, 2001)
4. 4. International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSBEP), OECD-NEA Nuclear Science Committee, NEA/NSC/DOC(95)03, September 2004 Edition.
5. 5. https://www.oecd-nea.org/science/wprs/shielding/sinbad/sinbadi.htm
   S.P. Simakov, B.V. Devkin, M.G. Kobozev, V.A. Talalaev (Inst. of Physics and Power Engineering, Obninsk),U. Fischer, U. von Moellendorff (Forschungszentrum Karlsruhe), Radiation shielding and dosimetry experiments database (SINBAD) , IPPE Fe shells Experiment and Analysis.

Appendix A. *RM* Standard Structure of Multichannel-Multilevel Resonance Parameters

LMF	Class identifier of the ENDF original data (MF)
KRM	Flag to specify which formulae for the R-matrix are to be used: =1 for single-level Breit-Wigner (SLBW) =2 for multilevel Breit-Wigner (MLBW) =3 for Reich-Moore (RM) =4 for full R-matrix
NISOT	Number of isotopes in the material
ISOT	Serial number of the current isotope
NJS	Number of *J* total angular momenta
IJS	Serial number of *J*
KIFG	Channel width representation flag: =0 - channel width in eV, =1 - reduced-width amplitude in $eV^{1/2}$.
KRL	Kinematics flag: nonrelativistic/relativistic (KRL=0/1)
NR	Number of reactions (particle pairs)
NCH	Number of channels
NRES	Number of resonances
KRB	Flag of background R matrix parameter representation: =0 – no terms are added to the R-matrix =1 – tabulated complex function of energy =2 – SAMMY's logarithmic parameterization =3 – Fröhner's parameterization
KSH	Flag of non-hard-sphere phase shift parameter representation: KSH=0 – hard-sphere phase shift, no additional information KSH=1 – phase shift is tabulated complex function of energy
LRB	Length of the RB array with background R matrix parameters
LSH	Length of SH array with phase shift representation parameters
LR(NR)	List of reactions (pair-particle identification numbers)
LZAR(2,NR)	List of charge values for particles in pair
LPNT(NR)	List of flags if penetrability is to be calculated: = 1 - calculate penetrability; = –1 - do not calculate penetrability; = 0 - assign value depending on the MT number; default value: = -1 for fission (MT=19) or capture (MT=102), = 1 for other MT numbers
LSHF(NR)	List of flags if shift factor is to be calculated: SHF=+1 calculate the shift factor; SHF=–1 do not calculate the shift factor
LRCH(NCH)	Particle-pair identification number for channel
LCH(NCH)	Values of orbital angular momenta *l*

NRB(4)	Descriptors of the RB array with background R matrix parameters: NRB(1) = number of points in real part of function NRB(2) = interpolation law for real part of function NRB(3) = number of points in imaginary part of function NRB(4) = interpolation law for imaginary part of function
KRBR(2,-NRB(2)	Interpolation table for real part of the background R matrix (NRB(2)<0)
KRBI(2,-NRB(4))	Interpolation table for imaginary part of the background R matrix (NRB(4)<0)
NSH(4)	Descriptors of the SH array with phase shift parameters NSH(1) = number of points in real part of function NSH(2) = interpolation law for real part of function NSH(3) = number of points in imaginary part of function NSH(4) = interpolation law for imaginary part of function
KSHR(2,-NSH(2))	Interpolation table for real part of the shift parameters (NSH(2)<0)
KSHI(2,-NSH(4))	Interpolation table for imaginary part of the shift parameters (NSH(4)<0)
EL	Lower limit of the energy range (eV)
EH	Upper limit of the energy range (eV)
EPS	Processing uncertainty (zero for evaluated data)
AW	Mass of the target nucleus (C^{12})
ABN	Abundance (a number fraction) of an isotope in the material
±SJ	Total moment *J* (spin); sign indicates parity
±PJ	Parity (used only if SJ=0.0): PJ=±1.0; sign indicates parity
AR(2,NR)	Mass of particles in pair (C^{12})
QR(NR)	*Q*-value for particle-pairs (eV)
SPR(4,NR)	SPR(1,IR) = spin of first particle in the IR-pair SPR(2,IR) = parity of first particle in the IR-pair SPR(3,IR) = spin of second particle in the IR-pair SPR(4,IR) = parity of second particle in the IR-pair
SCH(NCH)	Channel spin
BND(NCH)	Boundary condition for channel (needed when SHF=+1)
APE(NCH)	Effective channel radius (scattering radius), used for phase shift (10^{-12} cm)
APT(NCH)	True channel radius, used for calculation of penetrability and shift factors (10^{-12} cm)
RB(LRB)	Background R matrix parameters
SH(LSH)	Phase shift parameters
TAB(*)	Table of resonance parameters: (ER(IRES),(GR(ICH,IRES),ICH=1,NCH),IRES=1,NRES) ER – resonance energies (eV), GR – resonance widths (eV) or reduced-width amplitude ($eV^{1/2}$), depending from KIFG value (0 or 1)

Appendix B. Example of RML parameters output by the TABLE module

```
*******************************************************************************
Structure:*rm* MAT=2631 target: 026-Fe-056 projectile:   n
 lmf   - data class identifier.....................................          2
 nfor  - formalisms number.........................................          3
 nisot - number of isotopes........................................          1
 isot  - isotope serial number.....................................          1
 njs   - number of values of J.....................................          7
 ijs   - serial number of J........................................          1
 kifg  - flag of GAM: 0 - width in eV, 1 - reduced width.in.ev^1/2...          0
 krel  - flag for kinematics: 0 - non-relativistic, 1 - relativistic.          0
 nr    - total number of reaction (particle pairs).................          3
 nch   - number of chanals.........................................          4
 nrs   - number of resonances.....................................        111
 krb   - flag of background R matrix representation................          0
 ksh   - flag of non-hard-sphere phase shift representation.......          0
 lrb   - number of background R matrix parameters..................          0
 lsh   - number of phase shift parameters..........................          0

 el  - low limit of energy range (eV)............................. 1.000000-5
 eh  - upper limit of energy range (eV)........................... 2.000000+6
 eps - data uncertainty........................................... 0.000000+0
 aw  - target nucleus mass (C12).................................. 5.593494+1
 ab  - abundance.................................................. 1.000000+0
 sj  - J (spin)................................................... 5.000000-1
 pj  - parity (if sj=0)........................................... 0.000000+0

 Particle pair parameters ......
 ir   MT       Q         ZA   ZB      MA          MB          IA      IB   PNT  SHF
  1    2   0.000000+0    0   26  1.008665+0 5.593500+1   1/2+     0+    1    0
  2   51  -8.467778+5    0   26  1.008665+0 5.593500+1   1/2+     2+    1    0
  3  102   0.000000+0    0   26  0.000000+0 5.694366+1     1+     0     0    0

 Chanal parameters .....
 ic   MT   L      SCH         BND         APE         APT
  1    2   0  5.000000-1 0.000000+0 5.437300-1 5.437300-1
  2   51   2  1.500000+0 0.000000+0 7.515388-1 7.515388-1
  3   51   2  2.500000+0 0.000000+0 7.515388-1 7.515388-1
  4  102   0  0.000000+0 0.000000+0 0.000000+0 0.000000+0

             R-Matrix Limited formalisms
 J= 1/2+   Resonance Parameters
 ires    e0         gr=    2         51         51        102
    1 -1.263235+5 4.551305+4 0.000000+0 0.000000+0 1.000000+0
    2 -4.437377+4 6.247610+3 0.000000+0 0.000000+0 1.000000+0
    3 -2.461208+3 1.908200+2 0.000000+0 0.000000+0 9.063227-1
    4  2.779100+4 1.409300+3 0.000000+0 0.000000+0 8.600000-1
    5  7.402900+4 6.114601+2 0.000000+0 0.000000+0 5.900000-1
    6  8.362800+4 1.215100+3 0.000000+0 0.000000+0 5.400000-1
    7  1.298839+5 6.032718+2 0.000000+0 0.000000+0 5.700000-1
    8  1.405718+5 2.864369+3 0.000000+0 0.000000+0 1.580000+0
    9  1.693109+5 9.947203+2 0.000000+0 0.000000+0 1.000000+0
   10  1.878503+5 3.766206+3 0.000000+0 0.000000+0 1.020000+0
   11  2.206270+5 1.309228+3 0.000000+0 0.000000+0 1.680000+0
   12  2.450109+5 4.943092+2 0.000000+0 0.000000+0 6.000000-1
   13  2.772960+5 3.679982+3 0.000000+0 0.000000+0 8.000000-1
   14  3.180954+5 7.078331+3 0.000000+0 0.000000+0 9.200000-1
```

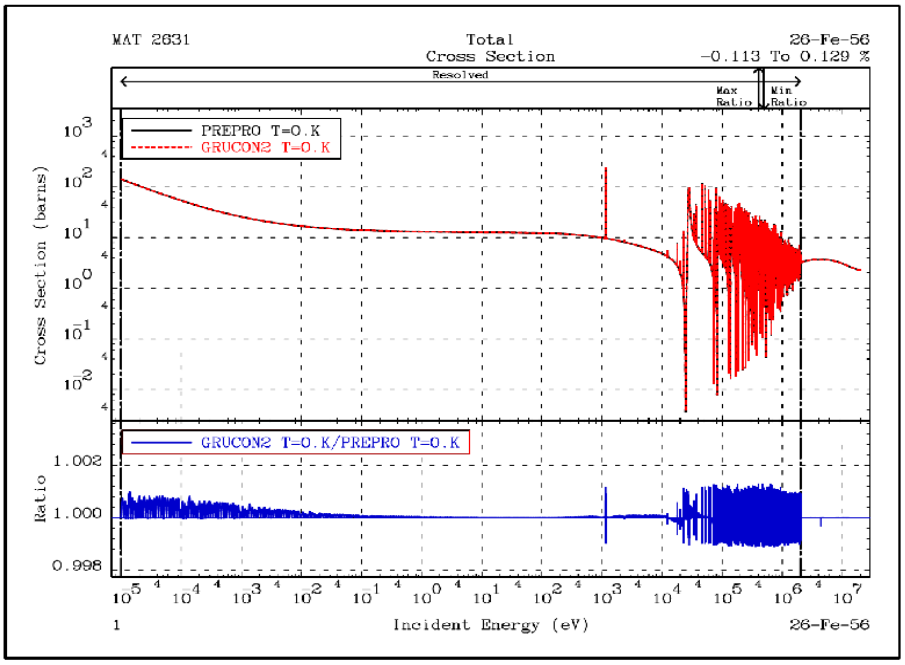
APENDIX C. GRUCON Input Task for the Verification Procedure

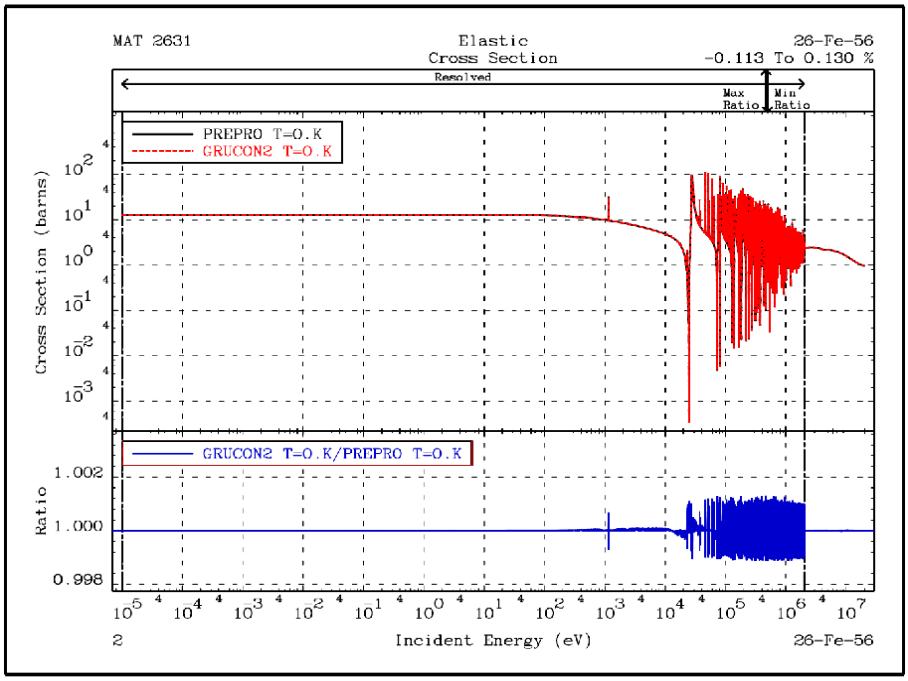
```
! Prepare point-wise  and group-wise cross sections
! for zero and room temperatures
,,,init,1,0,100000k
,,,init,2,0,1000000k
,,,init,3,0,1000000k
,in,,           ! enter local parameters
,in,1,endf      ! enter control parameters
,in,2,s/i-s
,in,3,extra     ! resonance cross section
,in,4,extra     ! (n,alpha)
,in,5,s/c-s
,in,6,s/a-s
,in,7,s/a-s
,in,8,s/a-s
,in,9,r/t-s
,in,10,u/d-s
,in,11,s/e-s
,in,12,s/t-s
,in,13,s/-s
,in,14,endf
,in,15,endf
,1,20,data       ! read endf tape
20,sel,21,*h*
20,sel,22,*nu*
20,sel,23,*rm*
20,sel,24,*u*
20,2,25,*s*      ! linearize tabulated cross sections
23,cp,25
24,cp,25
25,5,26,*s*        ! combain all tabulated cross sections
26,6,32,*s*,2      ! prepare background cross sections
23,9,33,*s*,3      ! reconstruct from resolved resonance parameters
24,10&25,33        ! reconstruct from unresolved resonance parameters
33,7,32            ! add resonance components to background
32,5,33,*s*        ! combine resonant cross sections
33,8,32,*s*        ! prepare nonelastic
32,11&25,33,*s*   ! thin
! prepare point cross sections at zero temperature
21,cp,32,*h*      ! copy *h*
23,cp,32          !      *r*
33,13,32          ! unpack resonant cross sections
25,3&1,32         ! add nonresonant cross sections
32,14&1           ! write cross sections for zero temperature
! prepare doppler broadened cross sections
33,12&25,32,*s*
32,11&25,33,*s*
```

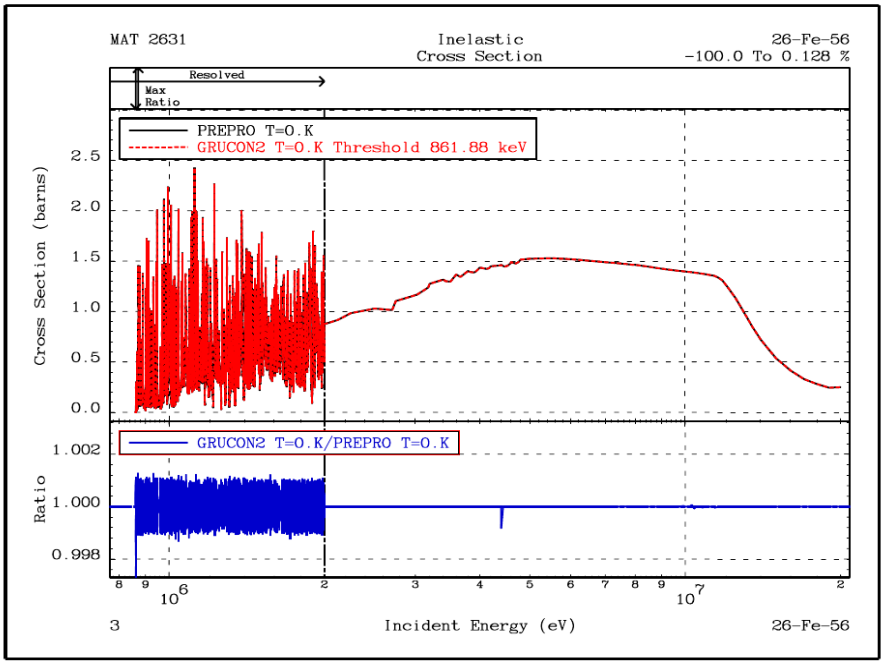
```
21,cp,32,*h*       ! copy *h*
23,cp,32           !      *r*
33,13,32           ! unpack
25,3&1,32          ! add nonresonant cross sections
32,15&1            ! write cross sections for given temperature
,,,end
! ------------ local parameters:
*de:1.e-5,1.5e8,
*/de:1.e-5,1.e1,
*nt:1,
*tem:293.6,
*eps:0.001
! ------------ control parameters:
*endf:ntape=20,nmat=0,nmf=3,nmt=4,mf=1,2,3,mt=1,2,5,-999
*s/i-s:nint=2,*de,*eps
*extra:ntyp=2,nmod=3,nr=7,lr=1,2,4,18,19,51,102
*extra:ntyp=2,nmod=3,nr=2,lr=107,800
*s/c-s:ncom=0,ns=0,*de,*eps
*s/a-s:nop=16,
 li=2,5,11,16,-18,22,-26,28,-37,41,-42,44,-45,50,-91,102,-112,2,50,-91,18,19,51,102,
 lo=1,1,1,1,1,1,1,1,1,1,2,4,18,19,51,102,
 lop=1,1,1,1,1,1,1,1,1,1,0,1,0,0,0,0
*s/a-s:nop=7,
 li=1,2,51,18,18,51,102,
 lo=1,2,4,18,19,51,102,
 lop=0,0,0,0,0,0,0
*s/a-s:nop=9,
 li=1,2,1,2,4,18,19,51,102,
 lo=1,2,3,3,4,18,19,51,102,
 lop=0,0,1,2,0,0,0,0,0
*r/t-s:nfor=0,nt=1,*de,*eps,tem=0.
*u/d-s:nfun=0,nin=2,nt=1,
      *de,*eps,tem=0.
*s/e-s:*eps
*s/t-s:*nt,*de,*eps,*tem
*s/-s:nr=0,nt=0
*endf:ntape=32,nmat=0,nmf=0,nmt=0
*endf:ntape=33,nmat=0,nmf=0,nmt=0
```

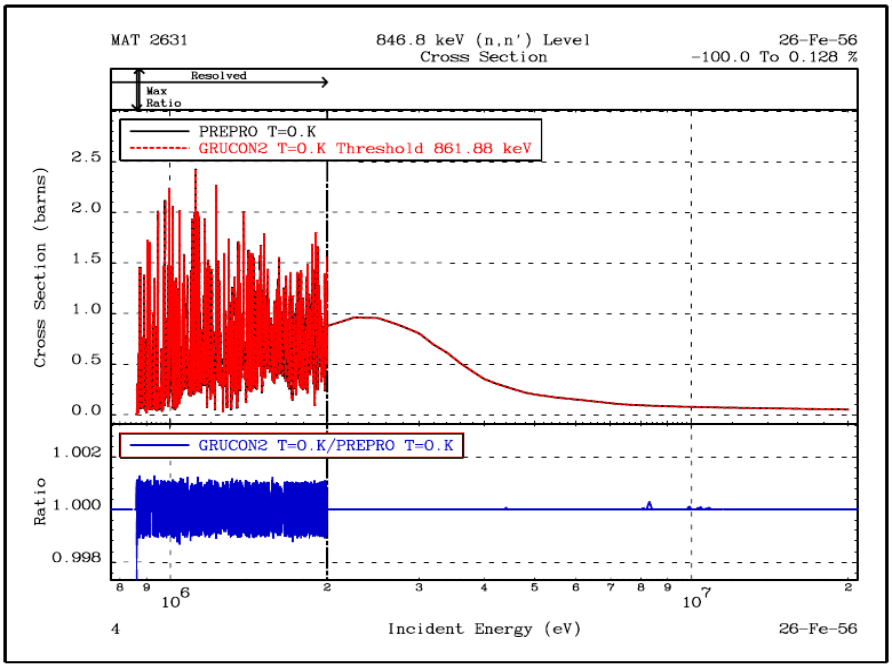
Appendix D. Verification Results: Comparison GRUCON vs. PREPRO

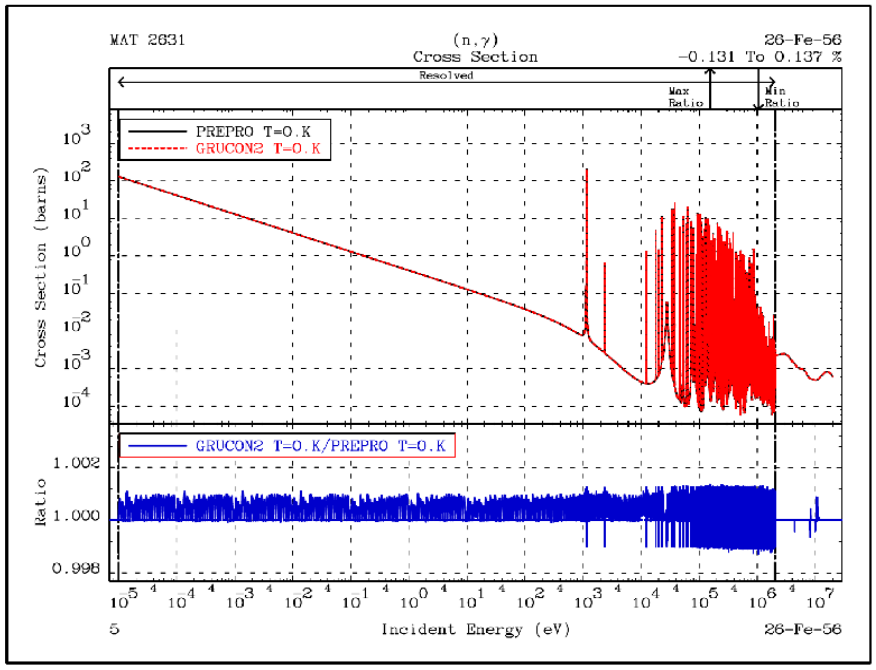
Temperature T=0K



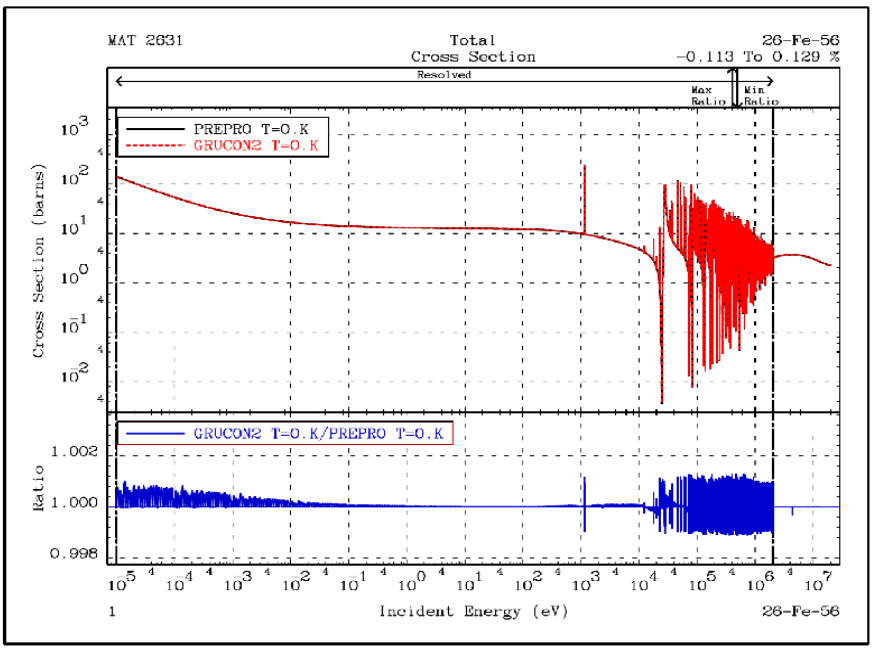


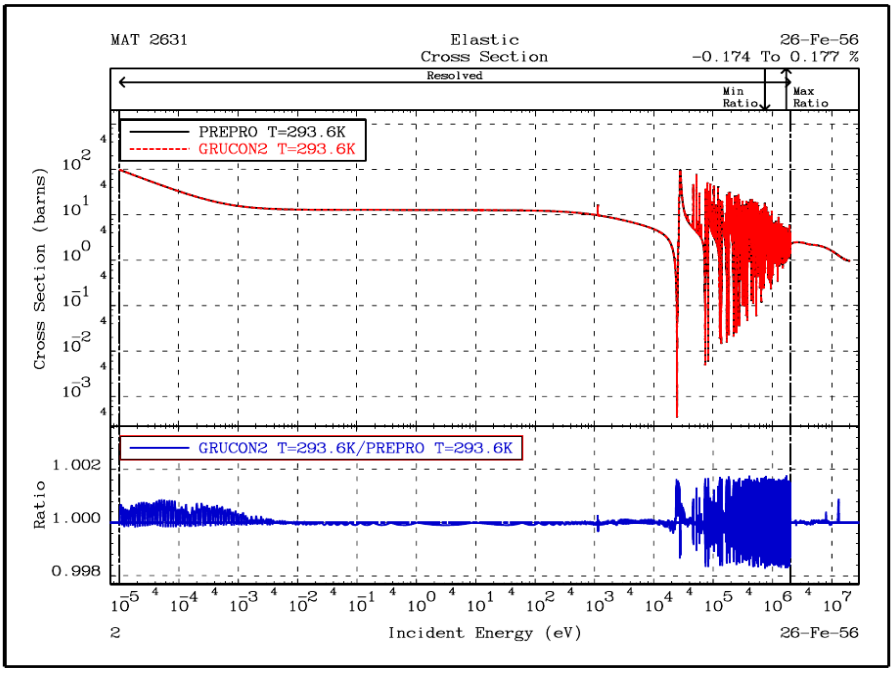

MAT 2631
Inelastic
Cross Section
26-Fe-56
-100.0 To 0.128 %
Resolved
Max
Ratio
PREPRO T=0.K
GRUCON2 T=0.K Threshold 861.88 keV
Cross Section (barns)
2.5
2.0
1.5
1.0
0.5
0.0
GRUCON2 T=0.K/PREPRO T=0.K
Ratio
1.002
1.000
0.998
8 9 10^6 2 3 4 5 6 7 8 9 10^7 2
3
Incident Energy (eV)
26-Fe-56

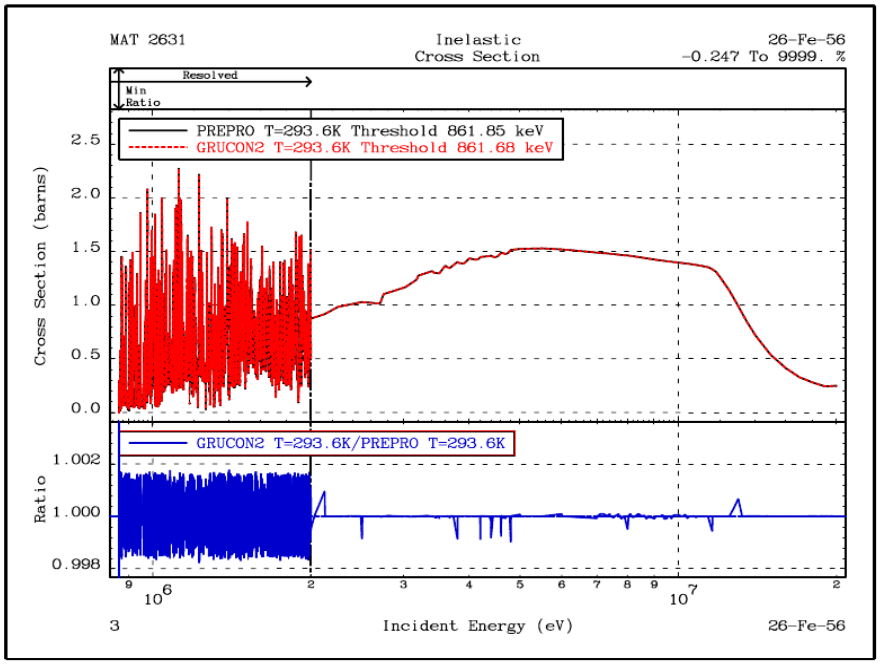

MAT 2631
846.8 keV (n,n') Level
Cross Section
26-Fe-56
-100.0 To 0.128 %
Resolved
Max
Ratio
PREPRO T=0.K
GRUCON2 T=0.K Threshold 861.88 keV
Cross Section (barns)
2.5
2.0
1.5
1.0
0.5
0.0
GRUCON2 T=0.K/PREPRO T=0.K
Ratio
1.002
1.000
0.998
8 9 10^6 2 3 4 5 6 7 8 9 10^7 2
4
Incident Energy (eV)
26-Fe-56

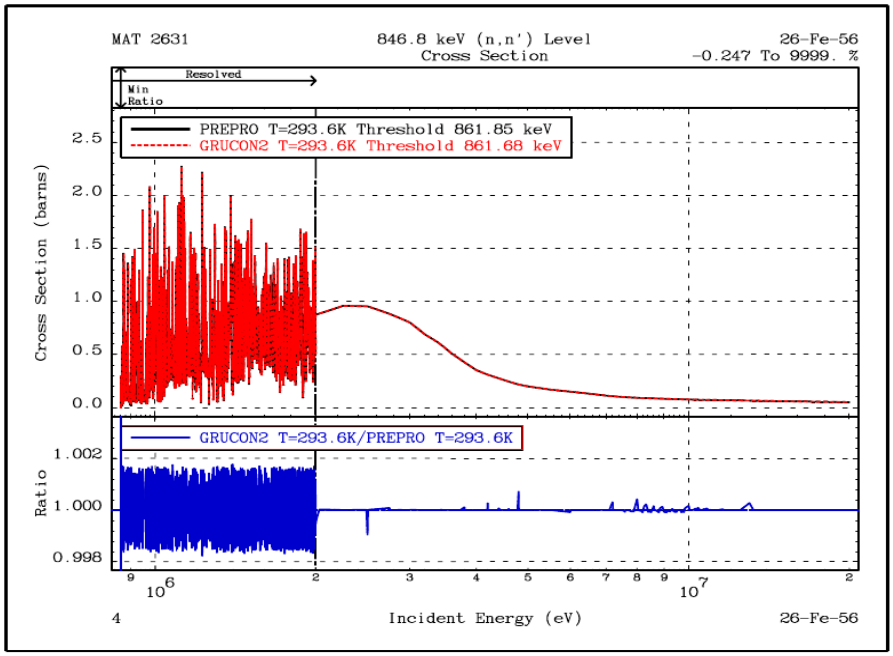

MAT 2631
(n,γ)
Cross Section
26-Fe-56
-0.131 To 0.137 %
Resolved
Max Ratio
Min Ratio
PREPRO T=0.K
GRUCON2 T=0.K
Cross Section (barns)
GRUCON2 T=0.K/PREPRO T=0.K
Ratio
1.002
1.000
0.998
Incident Energy (eV)
5
26-Fe-56

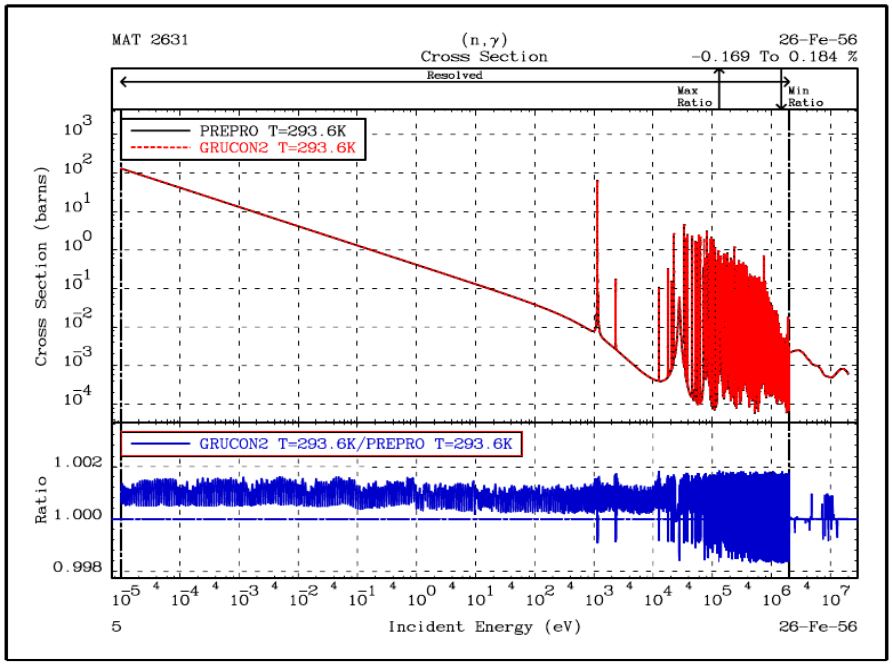
Temperature T=293.6K






MAT 2631
Inelastic
Cross Section
26-Fe-56
-0.247 To 9999. %
Resolved
Min
Ratio
PREPRO T=293.6K Threshold 861.85 keV
GRUCON2 T=293.6K Threshold 861.68 keV
Cross Section (barns)
2.5
2.0
1.5
1.0
0.5
0.0
GRUCON2 T=293.6K/PREPRO T=293.6K
Ratio
1.002
1.000
0.998
10^6
10^7
3
Incident Energy (eV)
26-Fe-56


MAT 2631
846.8 keV (n,n') Level
Cross Section
26-Fe-56
-0.247 To 9999. %
Resolved
Min
Ratio
PREPRO T=293.6K Threshold 861.85 keV
GRUCON2 T=293.6K Threshold 861.68 keV
Cross Section (barns)
2.5
2.0
1.5
1.0
0.5
0.0
GRUCON2 T=293.6K/PREPRO T=293.6K
Ratio
1.002
1.000
0.998
10^6
10^7
4
Incident Energy (eV)
26-Fe-56


MAT 2631
(n,γ)
Cross Section
26-Fe-56
-0.169 To 0.184 %
Resolved
Max Ratio
Min Ratio
PREPRO T=293.6K
GRUCON2 T=293.6K
Cross Section (barns)
GRUCON2 T=293.6K/PREPRO T=293.6K
Ratio
1.002
1.000
0.998
Incident Energy (eV)
5
26-Fe-56

Appendix E. Input task for ACE file generation

Fast Neutron

```
! Test 5: ACE file preparation
,,,init,1,0,10000k
,,,init,2,0,1000000k
,,,init,3,0,1000000k
,in            ! enter local parameters
,in,1,endf      ! enter control parameters
,in,2,s/i-s
,in,3,s/c-s
,in,4,s/a-s
,in,5,r/t-s
,in,6,u/d-s
,in,7,s/e-s
,in,8,s/t-s
,in,9,u/d-f
,in,10,f/c-f
,in,11,f/e-p
,in,12,extra
,in,13,ace
,1,20,data      ! read endf data
20,sel,21,*nu*
20,sel,22,*r*
20,sel,23,*u*
20,sel,24,*a*
20,sel,25,*e*
20,sel,26,*ae*
20,2&1,27,s     ! linearize cross sections with threshold energies correction
22,cp,27
23,cp,27
27,3,28,s       ! combine all cross sections
28,4,32,s,2     ! prepare background
22,5,32         ! reconstruct cross sections from resonance parameters
23,6&27,32      ! reconstruct cross sections from average resonance parameters
32,3,33,s,3     ! unite cross sections
33,7&27,32,s    ! thin energy grid points
32,8&27,33,s    ! doppler broaden
33,7&27,32,s    ! thin after broadening
27,12,32        ! add nonresonance cross sections
23,9,28,f       ! calculate cross section moments
28,10,29,f      ! collapse cross section moments
29,11,32        ! prepare and add subgroup parameters
21,cp,32        ! add nu-bar data
24,cp,32        ! add angular distributions
25,cp,32        ! add energy distributions
```

```
26,cp,32        ! select and add energy-angle distributions
32,con
32,13
,,,end
! ---------------------------------------
!    local parameters
*de:1.e-5,20.e6,
*/de:10.e6,20.e6,
*nt:1,
*tem:300.,
*nz1:1,
*sigz1:0.,
*nz:23,
*sigz:1.e-10,0.1,0.215,0.465,1.,2.15,4.65,10.,21.5,46.5,100.,215.,465.,
      1.e3,2.15e3,4.65e3,1.e4,2.15e4,4.65e4,1.e5,2.15e5,4.65e5,1.e6,
*eps:0.001
! ---------------------------------------
!    control parameters
*endf:ntape=20,nmat=0,nmf=6,nmt=0,mf=1,2,3,4,5,6
*s/i-s:nint=2,*de,*eps
*s/c-s:ncom=0,ns=0,*de,*eps
*s/a-s:nop=15,
 li=2,5,11,16,-18,22,-26,28,-37,41,-42,44,-45,50,-91,102,-999,2,18,102,-999,600,-649,800,-849,
 lo=1,1,1,1,1,1,1,1,1,1,2,18,102,103,107,
 lop=1,1,1,1,1,1,1,1,1,1,0,0,1,1,1
*r/t-s:nfor=0,nt=1,*de,*eps,tem=0.
*u/d-s:nfun=0,nin=2,nt=1,
      *de,*eps,tem=0.
*s/e-s:*eps
*s/t-s:*nt,*de,*eps,*tem
*u/d-f:nfor=0,nin=0,
     *nt,*nz1,nl=-5,nh=4,
     *de,*eps,*tem,*sigz1
*f/c-f:nfun=100,nmat=0,ns=0,*nz,nl=-2,nh=0,
     *de,*eps,tr=0.,*sigz
*f/e-p:kg=0,nsub=-3,ntyp=0,nmet=2,nopt=1,nset=0,nrel=1,kint=5,nmod=1,
      sigz=0.,1.e10,*eps
*extra:kdat=2,nmod=3,nr=-5,lr=1,2,18,51,102
*ace:nace=50,nxsd=51,ntyp=1,*nt,lr=0,nbin=16,iwt=1,*de,*tem
```

Thermal neutron (bound nuclei)

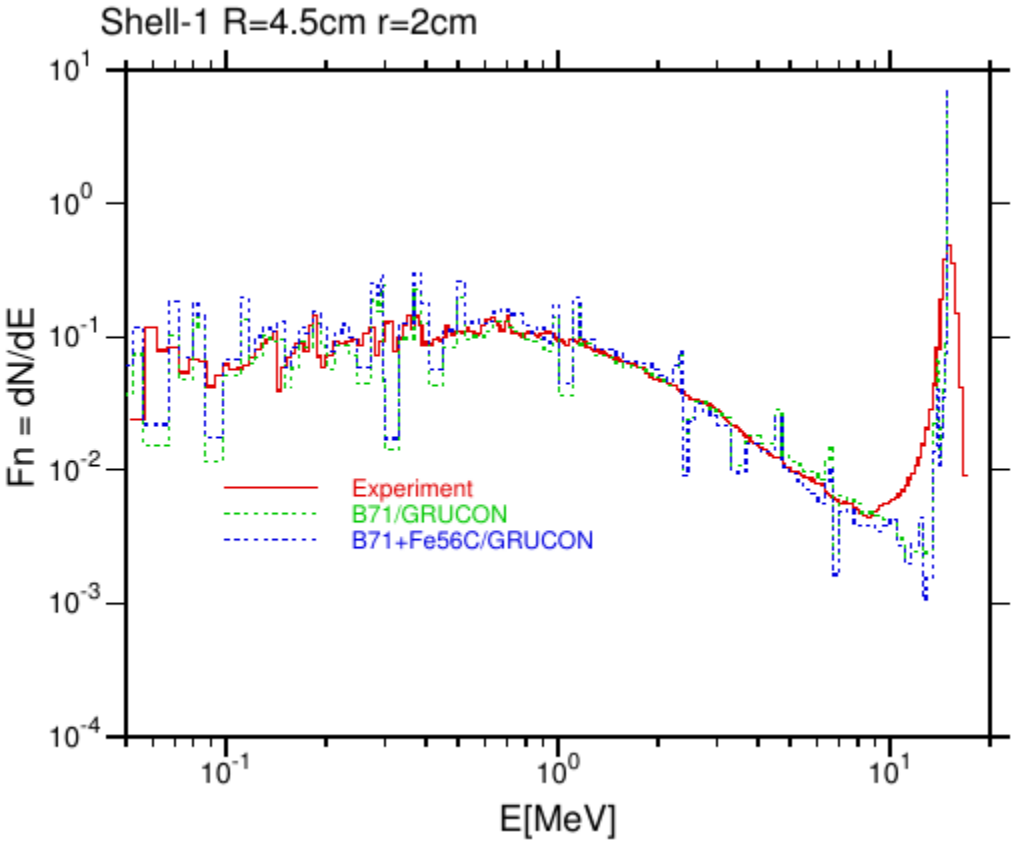
```
! Test 12: ACE file for thermal scattering on bound nuclei
,,,init,1,0,100000k
,in,,            ! enter local parameters
,in,1,endf       ! enter control parameters
,in,2,th/-ds     !
,in,3,ace        !
,1,20,*th*       ! read scattering law data from endf file
20,2,21,data     ! reconstruct differential cross section
21,3,,ENDF/B-VII.1! prepare ace file
,,,end
!------------------------------
!    local parameters
*mt:222,
*natom:2,
*de:1.e-5,4.65,
*nt:1,
*tem:293.6,
*eps:0.001
!------------------------------
!    control parameters
*endf:ntape=20,nmat=0,nmf=1,nmt=0,mf=7
*th/-ds:*mt,*natom,nint=2,nt=1,nang=32,ntypa=4,
      *de,*eps,*tem
*ace:nace=50,nxsd=51,ntyp=2,*nt,*mt,nbin=32,iwt=1,*de,*tem
```

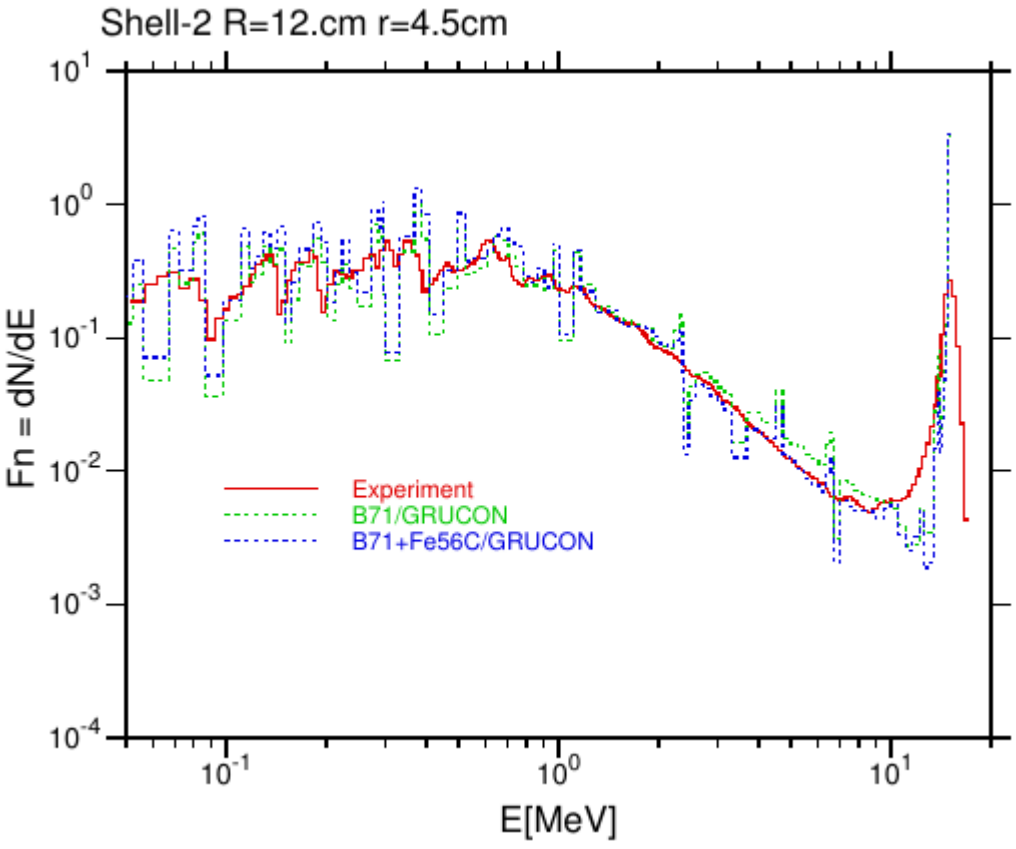
Appendix F. Keff Calculation for Critical Benchmark Experiments (ICSBEP)

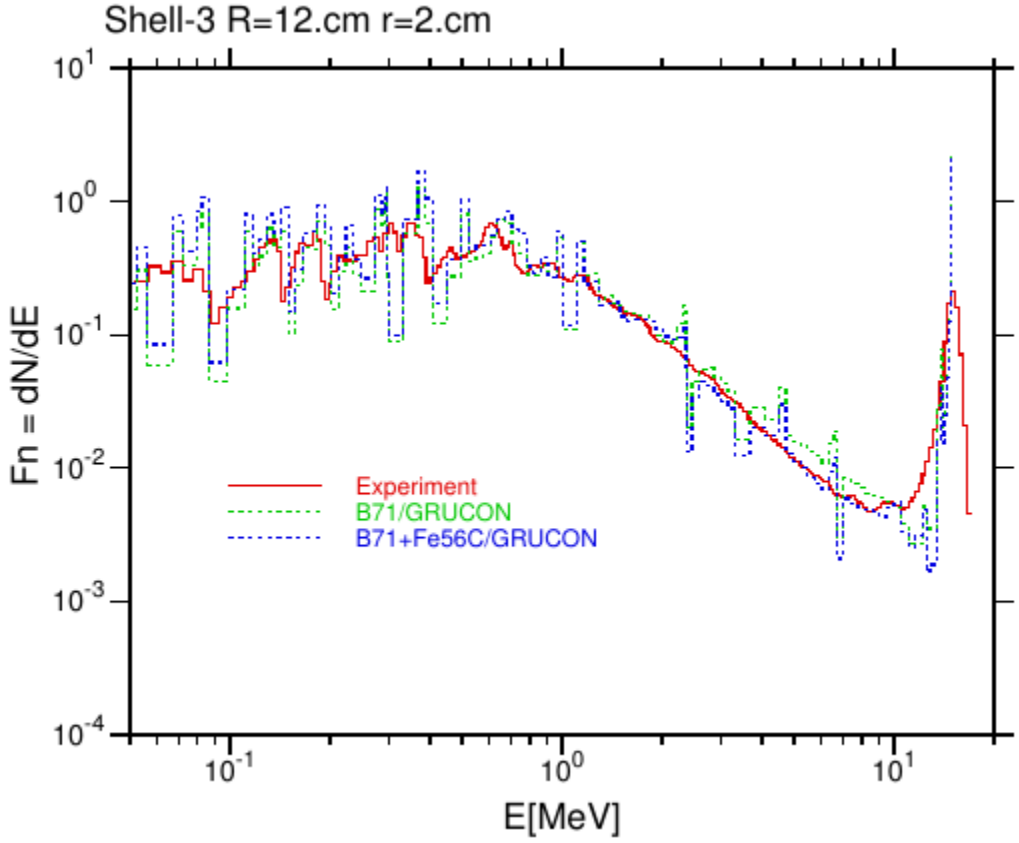
Benchmark		Experiment Keff	Experiment dKeff [pcm]	GRUCON/MCNP Keff	GRUCON/MCNP dKeff [pcm]
heu-met-fast-001	1,00000	100	1,00026	25	
heu-met-fast-002	1,00000	300	1,00212	29	
heu-met-fast-003_ni	1,00000	500	1,00916	30	
heu-met-fast-003_u1	1,00000	500	0,99526	28	
heu-met-fast-003_u2	1,00000	500	0,99516	28	
heu-met-fast-003_u3	1,00000	300	0,99963	28	
heu-met-fast-003_u4	1,00000	300	0,99775	29	
heu-met-fast-003_u5	1,00000	300	1,00212	31	
heu-met-fast-003_u6	1,00000	300	1,00212	29	
heu-met-fast-003_u7	1,00000	500	1,00201	30	
heu-met-fast-003_w1	1,00000	500	1,01838	28	
heu-met-fast-003_w2	1,00000	500	1,00217	27	
heu-met-fast-003_w3	1,00000	500	1,00609	28	
heu-met-fast-003_w4	1,00000	500	1,00961	29	
heu-met-fast-028	1,00000	300	1,00348	30	
ieu-met-fast-007d	1,00450	70	1,00528	24	
ieu-met-fast-007s	1,00450	70	1,00561	24	
ieu-met-fast-007h	0,99480	130	0,99602	22	
mix-met-fast-001	1,00000	160	0,99974	28	

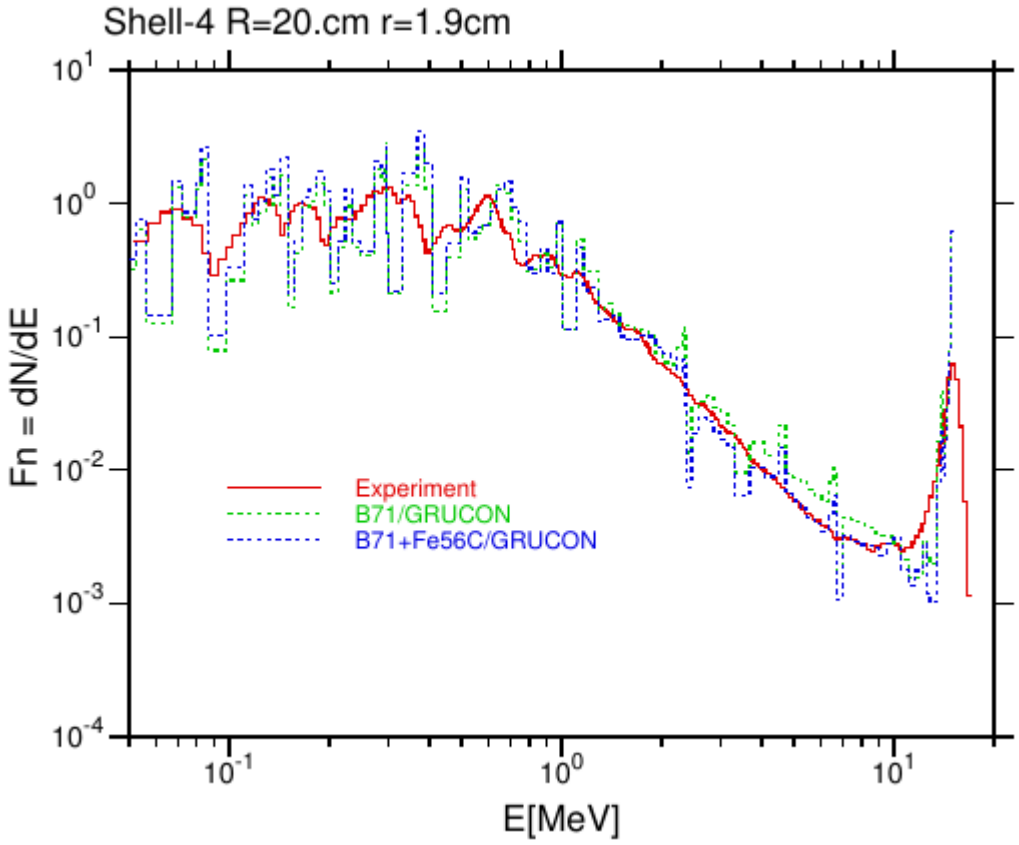
Benchmark		Experiment Keff	Experiment dKeff [pcm]	GRUCON/MCNP Keff	GRUCON/MCNP dKeff [pcm]
pu-met-fast-001	1,00000	200	1,00026	26	
pu-met-fast-002	1,00000	200	1,00035	25	
pu-met-fast-006	1,00000	300	1,00177	31	
pu-met-fast-008	1,00000	60	1,10721	60	
pu-met-fast-009	1,00000	270	0,99987	27	
pu-met-fast-010	1,00000	180	1,00046	28	
pu-met-fast-011	1,00000	100	1,00061	32	
pu-met-fast-023	1,00000	230	1,00038	28	
pu-sol-therm-006_1	1,00000	350	0,99999	34	
pu-sol-therm-006_2	1,00000	350	1,00077	33	
pu-sol-therm-006_3	1,00000	350	1,00012	33	
pu-sol-therm-011_16_1	1,00000	520	1,00947	41	
pu-sol-therm-011_16_2	1,00000	520	1,01368	41	
pu-sol-therm-011_16_3	1,00000	520	1,01566	41	
pu-sol-therm-011_16_4	1,00000	520	1,00862	41	
pu-sol-therm-011_16_5	1,00000	520	1,00569	42	
pu-sol-therm-011_18_1	1,00000	520	0,99284	34	
pu-sol-therm-011_18_2	1,00000	520	0,99916	34	
pu-sol-therm-011_18_3	1,00000	520	0,99567	35	
pu-sol-therm-011_18_4	1,00000	520	0,99213	37	
pu-sol-therm-011_18_5	1,00000	520	1,00235	35	
pu-sol-therm-011_18_6	1,00000	520	0,99908	39	
pu-sol-therm-011_18_7	1,00000	520	0,99925	34	
pu-sol-therm-021_7	1,00000	320	1,00549	41	
pu-sol-therm-021_8	1,00000	650	1,00304	42	
pu-sol-therm-021_9	1,00000	320	1,01346	41	
u233-met-fast-001	1,00000	100	0,99971	25	
u233-met-fast-002_1	1,00000	100	0,9987	26	
u233-met-fast-002_2	1,00000	110	1,00039	28	
u233-met-fast-003_1	1,00000	100	0,99922	27	
u233-met-fast-003_2	1,00000	100	0,99981	28	
u233-met-fast-006	1,00000	140	0,99938	30	

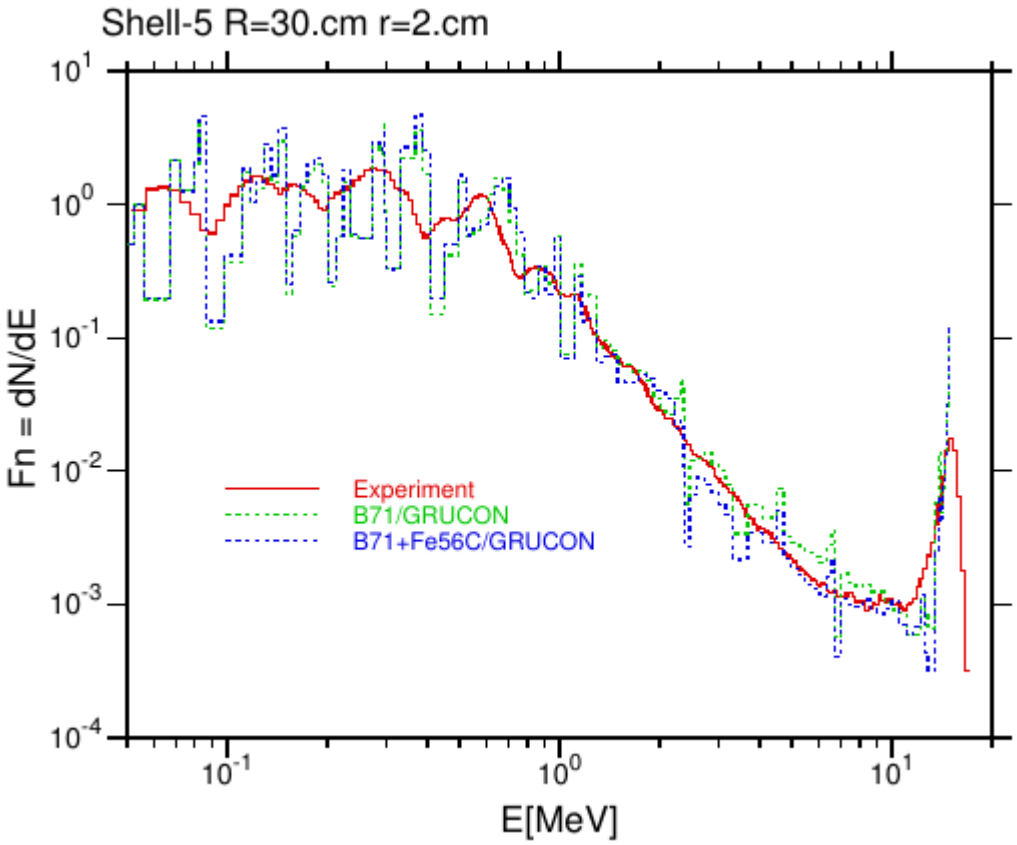
Appendix G. Leakage Spectra Calculation for Fe Spheres (SINBAD)






Shell-3 R=12.cm r=2.cm
Fn = dN/dE
E[MeV]
Experiment
B71/GRUCON
B71+Fe56C/GRUCON


Shell-4 R=20.cm r=1.9cm
Fn = dN/dE
E[MeV]
Experiment
B71/GRUCON
B71+Fe56C/GRUCON


Shell-5 R=30.cm r=2.cm
Fn = dN/dE
E[MeV]
Experiment
B71/GRUCON
B71+Fe56C/GRUCON

Conclusion