Benchmarking of the latest Neutron and Gamma Transport Cross Sections for Oxygen, Iron and Uranium in clean Benchmarks driven by D-T, $^{252}$Cf and Reactor sources

S.P. Simakov and U. Fischer

in collaboration with Experts from CIELO, JEFF, ....:
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**Nuclei Considered:**

I. **Oxygen:** our *(not completed yet)* validation results also presented as
   EFFDOC-13XX, NEA Data Bank, Nov 2017

II. **Iron:** a) continuation of our recent work *presented as*
    JEFFDOC-1851 = EFFDOC-1319, Apr 2017; EFFDOC-1303, Dec 2016

    b) MC propagation of TENDL-2017 random files to Covariancies
       for n & γ-leakage energy spectra *first time presented at*
       TALYS/TENDL Workshop, Nov 2017, Prague; then EFFDOC-13XX, Nov 2017

III. **Uranium:** revisiting our old validation *presented as a contribution to ND-2004*

*For these Nuclei following Evaluated Transport Data are under testing:*

- ENDF/B-VII.1 and ENDF/B-VIII.0 (= VIII.β4, CIELO)
- JEFF-3.3T4 and “JEFF-4.0T1” *(only 56Fe & 54Fe – L. Leal’ work for next JEFF)*
- TENDL-2017 evaluation and BMC random files *(only Fe stable isotopes)*

**Tools used:**
- File processing by NJOY-2012.82 (from LANL web) or .99 (NEA Data Bank)
- MC simulation of considered benchmarks by MCNP-6.1
  *(for TOF measurements: TOF was simulated then transformed to Energy Spectra)*
- dedicated f.95 subroutines for post processing of simulation results
I. Oxygen
## I. Oxygen (0): overview of Experiments with Liquid Oxygen involved in present analysis:

<table>
<thead>
<tr>
<th>Lab</th>
<th>Source: &lt;Energy&gt;</th>
<th>No. of Spheres: Wall Thickn., cm</th>
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**Additionals/Comments:**
- Liquid Oxygen Transmission experiment (En = 20 - 30 MeV) in progress at NPI/Rez, M. Majele et al. EFFDOC-1323, Apr 2017
- No gamma-leaking measurements! (then look what we have for water ?)

**Neutron scattering benchmark with pure Oxygen, NEA-1553/61:**

Neutron Leakage Spectra at 0, 12, 25, 42, 67 deg. from Liquid Oxygen Disc \((L = 20 \text{ cm} \times \varnothing 60 \text{ cm})\) irradiated by pulsed 14 MeV source

*Description of Experiment is available in:*
- e.g.: Y.Oyama et al., NDST 1991, p.337; Fig.3 =>
- Details & Numerical Data including author’s MCNP input - in SINBAD

*Essential experimental details which impact on modelling and conclusion:*
- measured by TOF which was also represented in MCNP simulations
- background was measured/subtracted by filling collimator hole with iron/polyethylene plugs
- efficiency of NE-213 detector was not measured but was MC-calculated by authors

*Our validation results of current evaluations on next slide (all O isotopes are included in MC)*
Findings: - **JEFF-3.3T4 = ENDF/B-VII.1** and **ENDF/B-VIII.0** are identical except ≈5% difference **only in 3 – 7 MeV**, where **ENDF/B-VIII.0** trends to unity.
I. Oxygen (2): LLL pulsed sphere with D-T source, 1967

**Observations:**

- **1st collision dominates**

- **ENDF/B-VII.1** is practically identical to **ENDF/B-VIII.0** however gives ≈2% more only for 4 - 8 MeV (similar to what we saw for FNS/JAERI slab)

- both confirm 14 MeV transmission but overpredict secondary neutrons 4-9 MeV (it similar as FNS shows at 0 - 25 deg)
I. Oxygen (3): ORNL, Tower Shielding Facility, 1967

Uncollided transmission through Liquid Oxygen
(length: 24in = 60.96 cm & 36in = 91.44 cm; dia: 4in = 10.16 cm)
irradiated by TSR-II reactor spectrum ranged 1.9 to 8.6 MeV

Description of Experiment is available in:
- e.g.: C.Clifford et al., NSE 27(1967)299; E.Straker ORNL-TM-2242(1968), -3868(1972)
- SINBAD NEA-1517/59: description + numerical data (only 60 in. = 152.4 cm), no MCNP model

Our preliminary results on next slide (all O isotopes are included in MC) =>
I. Oxygen (3): ORNL, Tower Shielding Facility, 1967 (cont.)

Observations but with preliminary set-up Model:

- This Reactor Spectrum Transmission Experiment indeed sensitive only to Uncollided Neutrons, i.e. to $\sigma_{tot}$:
  the fraction of Collided Neutrons seen by detector amounts only $\approx 5 \times 10^{-6}$

- It is insensitive to the change of Oxygen Temperature from boiling 90.2°K (-183°C) to room one:
  $\sigma_{tot}$ changes only below 1 eV

- 152 cm of liquid Oxygen reduce Neutrons by $10^{-4}$ !,
  $\Delta \sigma / \sigma = (n / \sigma)^{-1} \Delta T / T = 6.5 \Delta T / T$
  e.g.: 10% change of $\Delta T / T$ will demand $\Delta \sigma_{tot} \approx 0.65$ b !

- JEFF-3.3T4 is practically identical to ENDF/B-VII.1

- ENDF/B-VIII.0 gives 10% less then VII.1 only for 5-8 MeV or similar trend which we observe for FNS/JAERI slab and LLL sphere
II. Iron, the first part: Secondary Neutron Validation
### II. Iron (0): overview of Experiments involved in the present analysis:

<table>
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<tr>
<th>Lab Years</th>
<th>Source: &lt;Energy&gt;</th>
<th>No. of Spheres: Wall Thckn., cm</th>
<th>Method</th>
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<th>Numerical Data from</th>
</tr>
</thead>
<tbody>
<tr>
<td>IPPE 90-98</td>
<td>D-T: $\approx 14$ MeV</td>
<td>5 spheres: Wall = 2.5, 7.5, 10.0, 18.1, 28 cm</td>
<td>Time of Flight (TOF)</td>
<td>Neutrons: p-Ter.scint. &gt; 50 keV</td>
<td>S.Simakov et al. SINBAD Fusion: NEA-1553/75</td>
</tr>
<tr>
<td>IPPE 1985</td>
<td>$^{252}$Cf: $\approx 2.1$ MeV</td>
<td>6 spheres: Wall = 4, 9, 19, 23, 29, 34 cm</td>
<td>Pulse Height (PH)</td>
<td>Neutrons: H-prop. 5 – 700 keV Stilben 0.2 - 17 MeV Gammas: Stilben 0.4 - 10 MeV</td>
<td>L.Trykov et al. ICSBEP/DICE: ALARM-CF_FE_SHIELD-001</td>
</tr>
<tr>
<td>VNIITF 1991</td>
<td>D-T: $\approx 14$ MeV</td>
<td>1 sphere &amp; 1 semi-sphere: Wall = 5 cm</td>
<td>Time of Flight (TOF)</td>
<td>Neutrons: Stilben &gt; 0.25 MeV Gammas (e-Recoils): Stilben &gt; 0.35 MeV</td>
<td>A.Saukov et al. SINBAD Fusion: NEA-1517/74</td>
</tr>
</tbody>
</table>
II. Iron (1): Results for IPPE D-T pulsed sphere (Wall=28cm)

Neutron leakage

Observations for 14 MeV pulsed and thickest (Wall = 28 cm) sphere:
- JEFF-4.0T1 (Geel) is different from EFF-3.3T4 but comparable with it from view abs(C/E -1)
- ENDF/B-VIII.0 looks better than ENDF/VII.1
II. Iron (2): Comparison of IPPE (28cm) and LLL (22cm) spheres with D-T pulsed source: Neutron leakage

Observations from comparison of LLL (Wall = 22cm) and IPPE (Wall= 28 cm):

- LLL: Neutrons > 1.6 MeV (for convenience of comparison I converted original ToF spectra in Energy ones and folded with Gauss)
- IPPE: Neutrons > 0.1 MeV
- both: show similar C/E in overlapping energies, e.g. 4 - 10 MeV is overestimated by ENDF/VII.1, where ENDF/B-VIII.0 performs better
II. Iron (3): Results for IPPE Fe sphere (Wall=29 cm) + $^{252}$Cf(s.f.), Neutron Leakage

Before MCNP simulation we modified MCNP input given in ICSBEP/Alarm-Cf_Fe-Shield-001:
- $^{252}$Cf(s.f.) source neutron spectrum (given as Watt with Froehner parameters) was replaced by PFNS Standard (Mannhart evaluation), $v_p = 3.7590$
- and we added delayed neutrons ($v_d = 0.0086$) with DFNS spectrum from ENDF/B-VII.1

Observations from C/E comparison:
- JEFF-3.3T4 looks even more better than others
- possible reasons for underestimation ($\sigma_{tot}$, angular distribution ...) by ENDF/B-VIII.0 were studied
Observations:

JEFF-4.0T1 which adopts $^{56}\text{Fe}(n,n')$ either Perey’71 (ORNL) or Plompen’13 (Geel) are hardly distinguished by this benchmark.
II. Iron, the second part:
- Secondary Gammas Validation and
- problem of L.Trykov’ Benchmark (ALARM-CF_FE-SHIELD-001)

L. Trykov et al. Atom Energy, 98(2005)50 (highlighting by couloirs is my):
“The experimental fluxes of >0.8 MeV neutrons are, for the most part, greater than the computed values, and the fluxes of >0.35 MeV photons are also greater than the computed values. The differences reach a factor of 2–3“:

TABLE 2. Characteristics of the Neutron and Photon Spectra from Spherical Iron Models with a $^{252}$Cf Source at the Center

<table>
<thead>
<tr>
<th>Diameter of spherical model, cm</th>
<th>Flux of &gt;10 keV neutrons/source neutron</th>
<th>Flux of &gt;0.35 MeV photons/source neutron</th>
<th>Average energy of the photon spectrum, MeV</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Experiment</td>
<td>Calculation</td>
<td>Experiment</td>
</tr>
<tr>
<td>20</td>
<td>0.98</td>
<td>0.995</td>
<td>0.112</td>
</tr>
<tr>
<td>40</td>
<td>0.97</td>
<td>0.988</td>
<td>0.086</td>
</tr>
<tr>
<td>50</td>
<td>0.96</td>
<td>0.982</td>
<td>0.049</td>
</tr>
<tr>
<td>60</td>
<td>0.94</td>
<td>0.975</td>
<td>0.035</td>
</tr>
<tr>
<td>70</td>
<td>0.91</td>
<td>0.965</td>
<td>0.0165</td>
</tr>
</tbody>
</table>

What could be a reason for differences between L.Trykov experiment and calculations by factor 2–3 for leaking Gammas, when for leaking neutrons - it is within 10% (???)
II. Iron (1): IPPE bare $^{252}\text{Cf}$ source of Gammas vs. others

$^{252}\text{Cf(s.f.) Gamma Multiplicity: L.Trykov (ICSBEP, ...)}$ vs. other known data

Observations on Gamma to Neutron Multiplicities ratio Mg/Mn for $^{252}\text{Cf(s.f.)}$, $E_\gamma > 100$ keV:
- all known measurements (Cf fission chamber) and theory $\approx (8 - 10)/3.7676 = (2.1 - 2.7) – \text{it’s truth!}$
- Trykov/Alarm-Cf-Fe-Schield-001 (encapsulated Cf) $\approx (18 - 20)/3.7676 = (4.7 - 5.3) – \text{why?}$
Looking on these spectral data I did following:

1. from comparison of g-spectra \((E_g = 0.5 - 3 \text{ MeV})\) from L.Trykov’ bare Cf source (corrected for attenuation in CuFe capsule) and known PFGS there was found Normaliz. Factor \(= 0.33 \pm 20\%\)

2. this Factor was applied to all Iron g-leakage spectra measured by L.Trykov (all slides on next slides show his data after correction)

3. in MCNP input file the ABBN-93 g-spectrum was replaced by one derived from independent measured PFGS \(< 1 \text{ MeV}\) and P.Talou’ modelling \(> 1 \text{ MeV}\)

NB. Additional verifications of such correction against independent measurements of g-leakage from encapsulated Cf source and Fe spheres are highly needed
Observations/Comments on:

1. Distortion of \( ^{252}\text{Cf(s.f.)} \) Gamma Spectrum in Fe/Cu capsule:
   - below 7 MeV – attenuation by \( \approx 10\% \)
   - above 7 MeV – increasing by up to 50% due to \((n,\gamma)\) on Fe and Cu

2. above 5 MeV the \( ^{252}\text{Cf(s.f.)} \) \( \gamma \)-spectrum or L.Trykov’ bare source data seem are not so reliable - there we used P.Talou’ modelling since existing experimental PFGS data are controversial
Observations/Comments for Gamma leakage:
- No essential difference between JEFF-4.0T1, ENDF/B-VII.1 or ENDF/B-VIII.0
- but JEFF-3.3T4 lacks of high energy gammas from “thermal” (n,γ) on Fe-56 and Fe-54 as TENDL-2015/2017 do
II. Iron (1): Results for IPPE Fe sphere with $^{252}$Cf(s.f.), Neutron and Gamma Leakage vs. Wall Thickness

**Observations:**
- **Leaking Neutrons**
  - $0.1 - 1.5$ MeV – both ENDF/B-VII.1 and ENDF/B-VIII.0 are doing well
  - $1.5 - 10$ MeV – both lack removal XS
    - $= 60 \text{ mb (ENDF/B-VII.1)}$
    - $= 120 \text{ mb (ENDF/B-VIII.0)}$
- **Leaking Gammas**
  - status is worse than for neutrons
II. Iron (2): Independent DDX Measurements:
Fe(n,x) γ-production spectra at ≈2 and ≈7 MeV

Observation for differential Gamma spectra:
- Differential Experimental γ-ray production spectra for Fe(n,xy) reaction
  at neutron energies typical for Cf(s.f.) transmission benchmark
  do support the latest evaluations ENDF/B-VII.1, -VIII.0 and TENDL-2017
II. Iron (3): Independent Experiment for Gamma leakage:
VNIITF hemi- and spheres with D-T source

Observations for VNIITF’ Fe-sphere (Wall = 5 cm),
Leaking Gammas:
- whole sphere: ENDF/VII.1 looks almost perfect and better than ENDF/B-VIII.0
- back hemi-sphere: both ENDF/VII.1 and ENDF/B-VIII.0 overpredict by 30-150%
II. Iron, *the third part*:
straightforward Monte-Carlo propagation of Cross Section Uncertainties to Clean Benchmark Response Covariances
Propagation Method implemented:

- 1 + 500 TENDL-2017 Bayesian Monte Carlo (BMC) random files for each stable Fe isotope were provided by A.Koning and D.Rochman
- all were processed to ACE files by NJOY2012.82
- MCNP-6 simulation of neutron-gamma transport was re-run 1 + 500 times each run (1.E+9 events to reduce statistical uncertainty well below 1%) takes ≈ 3 min on 300 CPUs of KIT server
  total Wall time consumed was ≈ 16 hours (i.e., it is a feasible task !)
- neutron and gamma leakage spectra have been read-in from 501 MCNP output files to compute Covariancies Matrices

Example of Application:

- IPPE Iron sphere (R/r = 30/1cm, dia = 60 cm) with $^{252}$Cf(s.f.) source: results - on the next 2 slides =>
II. Iron: TENDL-2017 and Covariance propagation for IPPE Fe sphere with Cf source: Neutron Leakage

$n$ Leakage and Uncertainties $\approx 2$ - 20%

$n$ E-E Correlation Matrix: from strong correlation ($\approx 1$) to anti-correlation ($\approx -1$)

NB: Please note: original values are discrete points, colours are continuum interpolation between them!

Findings for n-Leakage: - Uncertainties ($\approx 2$-20%) from TENDL-2017 are comparable with Experimental - E-E correlations will play role below 100 keV, above 1 MeV – no correlation
Findings for $\gamma$-Leakage: - Uncertainties ($\approx 20$ - 40\%) from TENDL-2017 are comparable with Experimental
- TENDL-2017 underestimates Measurements: seem it lacks (n,\gamma) to ground state
- E-E correlations will play role in whole energy range 100 keV - 10 MeV
III. Uranium: Secondary Neutrons and Gammas Validation
### III. Uranium (0) – overview of Experiments involved in the present analysis:

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<td>IPPE 1998</td>
<td>(^{252})Cf: (\approx 2.1) MeV</td>
<td>1 sphere: Wall = 8.0 cm</td>
<td>Time of Flight (TOF)</td>
<td>Neutrons: Stilben 0.5 - 17 MeV</td>
<td>S.Simakov et al. AIP Conf. 769(2004)67</td>
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III. U (1): Results – Neutron Leakage from IPPE Sphere with D-T source

Neutron Leakage at 14 MeV

Observations:

*Both Spherical Benchmark and SED (dσ/dE) discover very similar trend:
- ENDF/B-VIII.0 underestimate 6-12 MeV interval
- ENDF/B-VII.1 looks better*
III. U (2): Results - Neutron leakage from IPPE sphere with $^{252}$Cf source

**Observations:**
- ENDF/B-VIII.0 and ENDF/B-VII.1 perform similarly well
III. U (3): Results - **Gamma leakage from VNIITF hemi- and whole spheres with D-T source**

**Observations:**

- first results – no conclusion yet, the experiment set-up models has to be checked
General Summary (details for each Nuclei - in proper sections)

- latest versions of ENDF, JEFF, TENDL evaluations for O, Fe and U are currently under validation against known clean benchmarks driven by neutron sources D-T, Cf and fast fields created at reactors
- quantities analyzed/tested are neutron and gamma leakage, uncollided neutron transmission
- relevant experimental benchmarks are available in SINBAD, ICSBEP or literature; however in some cases the complete information about measurements are not presented in these resources that prevent the correct modelling and concluding nowadays
- the main purposes of this work was to check whether independent benchmarks as well as differential XS indicate the similar trend for potential corrections/adjustments
- we generally saw this however excepting the case of L.Trykov’ measurements of \( \gamma \)-leakage from Iron spheres with Cf-source: \( \gamma \)-spectra seem have to be downscaled by factor \( \approx 3 \) to reach agreement with other differential and integral measurements (\( ? \) - still need confirmation! - additional independent measurements will be decisive)
- XS uncertainties (presented as TENDL-2017 randoms) were MC propagated to Covariancies of \( n \)- and \( \gamma \)-leakage spectra from Fe sphere fed by \( ^{252}\text{Cf} \)