

# INDC International Nuclear Data Committee

## Long-term International Collaboration to Improve Nuclear Data Evaluation and Evaluated Data Files

Summary Report of the Technical Meeting  
IAEA, Vienna, Austria  
18-21 December 2017

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National Nuclear Data Center, BNL  
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IAEA  
Vienna, Austria

March 2023

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## ABSTRACT

A summary is given of a Technical Meeting on “Long-term International Collaboration to Improve Nuclear Data Evaluation and Evaluated Data Files” at which participants assessed the need to establish an international network of nuclear data evaluation with the future medical applications for many radionuclides based upon their existing and potential diagnostic and therapeutic properties. Debate focused upon charged particle induced reactions and their production cross sections, derivation of optimal yields, minimization of radionuclidic impurities, and nuclear data needs for proton and heavy-ion radiotherapy, along with outstanding decay data requirements. Technical discussions are included in this report, along with comprehensive listings and detailed recommendations for future work. Required cross-section measurements were identified for a reasonably wide range of targets and projectiles, along with decay data studies for specific radionuclides. Subsequent excitation functions and decay-data evaluations will also be needed to ensure the necessary quality and consistency of the datasets to be assembled in an existing dedicated IAEA-NDS database that merits regular maintenance and support.

March 2023



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## 1 INTRODUCTION

The Technical Meeting on Long-term International Collaboration to Improve Nuclear Data Evaluation and Evaluated Data Files was held at the IAEA Headquarters from 19-21 December 2017. 29 participants from 12 countries and 2 International Organizations attended the meeting. The Section Head of the IAEA Nuclear Data Section, A. Koning, welcomed participants to the meeting on Monday morning while the Scientific Secretary, Roberto Capote Noy, reviewed the scope and goals of the meeting and highlighted the very successful CIELO collaboration organized by the NEA in Paris. R. Capote explained the idea of a new IAEA collaborative network - the International Nuclear Data Evaluation Network (INDEN). The new network will continue evaluation activities in the spirit of the NEA CIELO project, being the focus to improve the quality of evaluation methodology as well as of the evaluated data. In other words, we are interested in both the evaluation process as well as the results. The foreseen network could work through series of working yearly consultant meetings with ample allocated time for discussions of technical experts. Roberto also noted that experimental data are the main source of improvements in our evaluations, even if not included in the title. Therefore, those meetings will also cover the review of available data and discuss the needs for new measurements. We expect to have participants from all over the world including experts from the major nuclear data evaluation projects.

M. Herman was elected chairman and D. Brown and D. Rochman were designated rapporteurs. The preliminary agenda was adopted with changes and the meeting continued with presentations from participants, followed by technical discussions.

Summaries of the presentations are given in Section 2, while the technical discussions are described in Section 3. The Meeting Agenda and Participants list are available in Annexes 1 and 2, respectively. Links to the presentations are found in Annex 3.

## 2 PRESENTATION SUMMARIES

### 2.1 CIELO iron evaluation - lessons learned and vision of CIELO's future, M. Herman

Reviewed iron evaluation collaboration team, including BNL, RPI, JRC, CNDC, ORNL, IRSN, LANL, Brazil, KIT

Highlights of CIELO iron evaluation:

- In the resonance region we adopted basically F. Froehner's evaluation, with small improvements. Most important is the addition of background in famous capture window which was needed to reproduce RPI measurement around 24 keV, on natFe from Bob Spencer. In addition, fixed energy shift in one of resonances (at 28 keV).
- (n,inel) adopted experimental re-analysis from CNDC. The new CIELO evaluation is now somewhat lower than the "new" Nelson data (2004, but recently reworked by LANL).
- Fast neutron range cross sections: take IRDFF data if available but reproducing IRDFF evaluations with EMPIRE calculations so that all reactions are internally consistent.
  - A. Wallner (n,2n) measurement agrees with evaluation even though not used in fit; is a slight increase over VII.1;
  - (n, $\alpha$ ) not in evaluation because of disagreements between ENDF format and EMPIRE code, but derived alpha production data reproduced;
- Elastic angular distributions: good agreement on average, but fluctuations extend to very high in energy, so exact agreement is tricky. The CIELO evaluation fits Perey and Kinney data and used at low energy (< 4 MeV) and at high energy use EMPIRE (>4 MeV).

- DE and DEA spectra overall have good agreement.

#### Testing of CIELO iron evaluation:

- Overall reasonable agreement in ICSBEP benchmarks, slightly better than ENDF/B-VII.1 in most cases, a lot better PMI-002, HMF-088. Problems with agreement in many cases driven by other evaluations not in the scope of the CIELO project.
- Transmission experiment validation:
  - d-t source through iron sphere: neutron transmission much better, but imperfect;
  - $^{252}\text{Cf}$  source through iron sphere: neutron transmission better, but imperfect;
  - $^{252}\text{Cf}$  source, again: game transmission is much worse;
  - $^{252}\text{Cf}$ , neutron source energy determined from a spectrum unfolding — points to problem in (n,el), cross section may be too low or not enough forward peaked, but there is no sensitivity study to tell for sure.

#### Other results published after iron evaluation has been completed:

- AD from U. Kentucky (Ramirez);
- Rediscovery of AD data from Cierjacks;
- Renormalization of Nelson data;
- New 15% lower (n, $\gamma$ ) thermal point from Firestone;
- New Wallner (n,2n);

#### Things that clearly need improvement in the iron evaluation:

- New elastic scattering data from nELBE and GELINA show elastic cross section is low;
- Reconsider elastic/inelastic ratio. Comment from M. White on Nelson renormalization: no new resources;
- Need new resonance evaluation!
  - New resonance data,
  - Use LRF=7 if possible so can include (n,inel) in resonance region,
  - Attempt to eliminate background,
  - EGAF thermal capture point commented by A. Trkov: shall we trust Firestone's new evaluation?
  - Angular distributions from resonance parameters.
- Sensitivities in some benchmarks indicate that Ni and Cr may also have an impact;
- Proposal by Mike: continue Fe6 evaluation, and add Cr, Ni;

#### CIELO benefits:

- More efficient use of expertise;
- Experience sharing;
- Wider scrutiny (although would be better to happen at an earlier stage);
- More integral testing than we could do ourselves;
- Regular flow of information between projects;
- More visibility and weight:
  - More experiments fielded,
  - Collaboration with EXFOR,
  - Upper management likes it.

#### Comments on experimental data:

- Some data are only available in EXFOR as they have never been published.
- Four most important sets for Fe have never been published.



- Proprietary information tricky — must be cleared by sponsor before we can use, so we may know there is a problem with the evaluation, but we cannot do anything about it because data is embargoed. It is ironic, because until sponsor gets evaluation, they can't use it!
- A comment on this last point: if preliminary data are used, must be prepared to re-do evaluation as data is reworked prior to publication.

Dice sensitivities essential to pointing us in the right direction! NDaST might also be useful to simplify benchmarking.

Future strategy?

- Most important materials left behind by CIELO-1
  - Need user input
  - HPRL
  - Other user priority lists
- Materials correlated with CIELO-1 (Cr, Ni, ...)
- Should we expand CIELO beyond neutron sublibrary?
- We are stretched very thin....

CIELO-1 depended on differential data but calibrating to integral data means coupling materials and reactions.

Also, validation needs to happen continuously, so we always know where we are:

- ADVANCE possibility, but needs automatic benchmarking extension;
- NDaST also possibility, only linear response (but is FAST);
- Both need some kind of shared repository (git/svn for ADVANCE, MySQL for NDaST);
- Need to address deep penetration and shielding benchmarks;
- Question O. Iwamoto: different calibration from different libraries will lead to different results.

Evaluation needs to be preserved, so EVERYTHING can be repeated: procedures, data, renormalizations, etc.

Need for cross observable (cross-MF) correlations, e.g. in elastic. In this way we can correlate  $P_0, P_1, P_2 \dots$ . However, we can't process them! For fission, the situation is much worse.

## 2.2 Benchmarking of the latest neutron and gamma transport cross sections for oxygen, iron and uranium in the clean benchmarks driven by d-t and $^{252}\text{Cf}$ sources, S. Simakov

### Oxygen

- FNS/JAERI (ToF), 20 cm cylinder, in SINBAD
  - D-t source;
  - All libraries agree at larger angles and disagree with experiment (50 keV-10 MeV);
  - Suggests problem with experiment, not good agreement below 1 MeV (PSD is difficult, no exp. difference between gamma and neutrons);
  - Disentangling neutron from gamma below few MeV in this kind of experiment is difficult; This is why LLNL picked higher detector threshold.
- LLNL Pulsed Sphere (ToF), 10 cm sphere
  - D-t source;
  - ENDF libraries agree, but disagree with experiment from 4-10 MeV;
  - Inelastic scattering problem;

- Model built from Wong 1971? and Hansen 1976? (check refs.);
- Room return is an issue and no one knows the floor height....
- ORNL (Pulsed Height), cylinders of varying length, in SINBAD
  - Reactor spectrum through liquid oxygen;
  - TSR-II reactor;
  - Unfolding to get distribution;
  - No MCNP model, so had to make one;
  - Insensitive to temperature;
  - Big differences between ENDF 7 & 8 & experiment;
  - $(n,\alpha)$  decreased (less absorption), in contradiction with the ORNL results.
- In progress NPI/Rez EFFDOC-1323
- No gamma leakage measurements
- Common discrepancy suggests issue with DEA about 2-3 MeV

### Iron

- IPPE (90-98) d-t, sphere
- IPPE (1985)  $^{252}\text{Cf}$ , sphere
- LLNL (1976) d-t, 3 spheres
- LLNL (1990) d-t, sphere
- VNIITF (1991) d-t, sphere
- Fe IPPE + Cf, neutron leakage: B8 better than B71, but JEFF33 is also quite good (better ?)
- Common issues in 2-6 MeV suggests issue with elastic data, but is much reduced in B-8/CIELO compared to B-7
- Gamma leakage is bigger problem in B-8/CIELO. JEFF-3.3T4 is in better shape.
- Secondary gamma validation: L.A. Trykov Atom. Energy 98 (2005) 50, difference of factor 2-3! Is it an issue with the  $^{252}\text{Cf}$  gamma spectrum? Trykov measurements 2-3 times more than all other measurements. Suspicion is that there is roughly a factor of 3 normalization error in Trykov data.
- Systematic disagreement between calculated and experiment as a function of wall thickness with IPPE Fe benchmarks for leaked gammas, but not for neutrons. However, disagreement with thin wall (basically bare  $^{252}\text{Cf}$  source), suggesting that there is a problem with the source characterization w.r.t. gammas emitted.
- TENDL 500 random files used in IPPE Fe benchmarks. Leaked neutron spectra have similar shape to CIELO, but because of the 500 Monte-Carlo files, get uncertainties. Since TENDL has basically no capture cross section above 6 MeV, the gamma leakage is very low there.

### Uranium

- IPPE DU spheres with d-t source
  - ENDF/B-VIII.0/CIELO is quite low in the inelastic dip, just lower energy from elastic peak
  - 6-10 MeV, 70% of experiment
  - ENDF/VII.1 did not have this problem
  - There is a suspicion of the angle of the detector and hence an issue with the angular distribution, but data is angle integrated
  - ToF
- IPPE DU spheres with  $^{252}\text{Cf}$  source
- VNITF (probably DU) sphere
  - Slight underestimate of gamma leakage

## 2.3 Comments on CIELO project and future work, M. Chadwick

Continued work on CIELO is justified by success of previous project. International collaboration is essential as it is the only way to bring together required expertise.

We have found a completely new solution to criticality, achieving good benchmark results with new evaluation.

Principal directions we need to head in:

- Continued progress on main CIELO isotopes, work here is not done though. Potential deficiencies:
  - Elastic and inelastic scattering
  - Covariances were late and are incomplete: significant differences between subject matter experts and what is in files, need more consensus
- Consider more nuclei: deuterium, other actinides ( $^{233}\text{U}$ , Am, Cm,  $^{240}\text{Pu}$ )

Rapidly improving tools (optimization and automation), allows for faster turn-around.

CIELO paper has a section on main conclusion and findings.

We have not yet had a discussion as to what to tackle next. Should we use what experiments are done to guide us? Should we use sensitivities or perhaps the HPRL? Should we use our best judgement?

New experiments on actinides:

- PFNS experiments by CEA and LANL
- TPC now has fission data

Experiments that improve accuracy, even in a well-known area, help. Capture is one area where the impact will be great.

Current WPEC investigating capture on  $^{241}\text{Am}$ ,  $^{237}\text{Np}$ .

Semi-integral experiments give us new scheme for data testing. It is not clear whether improvements to current CIELO demonstrated improvement against these tests.

We have shown that we can turn around a benchmark in hours. We have not yet taken full advantage of sensitivity tools at NEA nor can we get feedback of testing back to the evaluators (within that few hour window) except in a few cases.

## 2.4 Improvements in the neutrons cross section evaluations, V. Pronyaev

Nubar

- prompt yields in resonance range
  - imprint of  $(n,\gamma f)$  in  $^{239}\text{Pu}$ , what about other actinides?
  - In between resonance dips, should nubar return average or something else.
- In region of max PFNS
  - Nubar and  $(n,2n)$  cross section measured by Frehaut with large liquid gadolinium detector relative to  $^{252}\text{Cf}(sf)$ . “Frehaut factor” of 7-8% applied to  $(n,2n)$ . Have they been applied to nubar? Frehaut’s nubar measurements done at PFNS energies.

## PFNS

- Below 700 keV
  - Differences between  $^{239}\text{Pu}$  ratio-to- $^{252}\text{Cf}(\text{sf})$  data and the evaluation, especially to Starostov data. Pu PFNS not updated in CIELO;
  - Good agreement between new Kornilov data and CIELO PFNS for  $^{235}\text{U}$ ;
  - May see impact in thermal solution benchmarks.
- Above fission chance thresholds
  - Vorobjev PFNS above 700 keV has large uncertainty.

Kudos to NEA for DICE!

## Elastic scattering angular distributions in the RR and cross section fluctuations

- Effect of the RRR detailed angular distribution is still inconclusive;
- Need mono isotopic reflector experiments with different thicknesses;
- Subgroup 35 still has not produced the final report.

## Interplay of elastic and inelastic

- Impacts of gamma production cross sections;
- Likely true for  $^{56}\text{Fe}$ , Geel data not completely exploited in the CIELO evaluation
  - Differences between Geel, Dresden and Nelson. Dickenson (ORNL) agrees with Geel
  - Clearly hard to disentangle and the disagreement impacts the shielding benchmarks;
- For  $^{238}\text{U}$  also probably true;
- Below 1 MeV in  $^{56}\text{Fe}$  — doorway states and multichannel coupling.

## Capture cross section for first resonances in even-odd nuclei of structural materials

- May have small natural abundance, but may be dominant contribution to capture in keV region;
- $^{53}\text{Cr}$  is typical case;
- HCI-005 has big sensitivity to  $^{53}\text{Cr}$ .

## 2.5 Lessons learned from CIELO evaluations and experimental needs, R. Capote

### Introduction:

- Rumsfeld: known-knowns & known-unknowns, but there are also unknown-unknowns;
- Why did we get small uncertainties in previous standards evaluations?
- If use same type of ruler, will get same systematic error even if each ruler is independent. This is true also for benchmarks, cross section measurements, etc. It is of course a property of the measuring tool/technique;
- Can we estimate unknown-unknowns? Basically, estimate the size of systematic errors from the measured data?

### $^{252}\text{Cf}(\text{sf})$ nubar

- 15 measurements, should the uncertainty shrink by  $\sqrt{15}$ ?
  - GMA gets 0.13% uncertainty with simple GLSQR fit
  - However, each measurement on its own has uncertainty 0.6%
  - $0.13 = 0.6/\sqrt{15}$
- Are the experiments truly independent?
- If so, then final PDF should be consistent with measured experiments
  - Assessment of minimum possible uncertainty;
- USU nubar is 0.4%?

Unrecognized systematic uncertainty assessed on standards reaction cross sections.

- One uncertainty for each light reaction, not energy dependent;
- May not be good approximation for  $^{197}\text{Au}(n,\gamma)$ ,  $^{238}\text{U}(n,\gamma)$  or  $^{235}\text{U}(n,f)$ .

Re-evaluation and/or experimental needs

- E. Pirovano et al. JRC Geel and nELBE measurement of  $^{\text{nat}}\text{Fe}(n,\text{el})$  (Ph.D. thesis)
- $^6\text{Li}(n,t)^4\text{He}$  differs from Standards 2016 to Standards 2017, well outside uncertainties of two evaluations
- Similar  $^{\text{nat}}\text{C}(n,\text{el})$
- All Li-glass uses maybe needs re-investigation
- Thermal constants added to standards, including  $^{235}\text{U}$ ,  $^{239}\text{Pu}$  (n,f) and (n,g); Needs experimental confirmation, especially fissile alpha below 5 eV
- Nubar fluctuations were added to  $^{235}\text{U}$ , no nubar uncertainties in large energy range, including region where we expect fluctuations; uncertainty large from 0.1-20 keV
- $^{235}\text{U}(n,\text{inel})$ ,  $^{238}\text{U}(n,\text{inel})$  big difference between JEFF-3.3T3 and CIELO; only way to make progress is to measure the internal conversion electron from first excited state(s). Need 8-10% uncertainty.
- $^{235}\text{U}$  in URR, mostly untouched. Above this, follow fluctuations in the data. Is this the right thing to do? Potential for “double counting” fluctuations in URR exists.
- PFNS normalization constraint means that we do not follow all the data, especially at low outgoing energy. Maybe experimental problem because of multiple scattering.

## 2.6 Foreseen experimental activities at CNRS-IN2P3 related to nuclear energy researches (2018-2021 and beyond), M. Kerveno

Overview of experimental activities & capabilities

IN2P3 is CNRS 6 teams in 6 laboratories Subatech, INP, CENBG, LPSC, IPHC, IPC-Cean; universities and high schools, 20 researchers, 12 from laboratories. Since 1996. CHANDA funding & NEEDS project. Also NACRE(CEA/IN2P3-Univ.-High School/IRSN).

Interested in ADS & various reactor scenario simulations.

Classes of measurements

- Cross section measurements
- Fission product measurements
- Fission product decay studies

All related to Gen—3 & 4 reactors, U/Pu and Th/U fuel cycles. Wish to become involved in evaluation process.

Planned experiments for next 3 years

- GRAPhEME setup to do prompt  $\gamma$ -ray spectroscopy
  - Several  $(n,n'\gamma)$  and some  $(n,2n\gamma)$ ,  $(n,3n\gamma)$
  - Final publication on  $^{\text{nat},182,183,184,186}\text{W}$ ,  $^{232}\text{Th}$  and  $^{238}\text{U}$
  - Measurement campaign  $^{233}\text{U}$
  - $^{239}\text{Pu}$
  - Collaboration with CEA/DAM theorists for  $(n,xn)\sigma$  determination
- $^{19}\text{F}(n,\alpha)^{14}\text{N}$  at 2.5 and 14.2 MeV planned for GENESIS/LPSC in 2018
- $\sigma$  measurements of  $^{19}\text{F}(n,\alpha)^{14}\text{N}$  and  $^{16}\text{O}(n,\alpha)^{13}\text{C}$  from threshold up to 20 MeV at SPIRAL2-NFS
- $^{231}\text{Pa}(n,f)$  at CERN-nToF, ratio of fission  $\sigma\sim 3\%$ , angular distributions
  - Final publication of  $^{237}\text{Np}$
  - $^{231}\text{Pa}$  in 2018 at EARS

- $^{240}\text{Pu}(^3\text{He}, ^3\text{He}')^{240}\text{Pu}$  Tandem-IPNO surrogate measurements at CENBG
  - $^{238}\text{U}(^3\text{He}, ^4\text{He})^{237}\text{U}$ ,  $^{238}\text{U}(^3\text{He}, t)^{237}\text{Np}$ ,  $^{238}\text{U}(^3\text{He}, d)^{238}\text{Np}$  publications in preparation, for  $n+^{236}\text{U}$ ,  $n+^{237}\text{Np}$  and  $n+^{238}\text{Np}$
  - $^{240}\text{Pu}(^4\text{He}, ^4\text{He}')^{240}\text{Pu}$ ,  $^{240}\text{Pu}(^3\text{He}, ^4\text{He}')^{239}\text{Pu}$  and  $^{240}\text{Pu}(^4\text{He}, ^3\text{He}')^{241}\text{Pu}$  planned
  - Collaboration with CEA/DAM, CEA/DEN, Jutta Escher @LLNL
- Grenoble ILL Lohengrin spectrometer:
  - Measurement of FP mass & isotopic yields and isomeric ratios
  - $^{241}\text{Pu}(n_{\text{th}}, f)$  absolute measurements
  - In future want isotopic and isomeric ratio for  $^{233,235}\text{U}$  and  $^{239,241}\text{Pu}$
  - Fission yield evaluation for major actinides
- SOFIA-GSI measure mass and change of both FF
  - Mass yields and TKE
  - $^{236}\text{U}$ , and neutron deficient pre-actinides
  - Neutron & fission fragment in coincidence
  - $^{180}\text{Hg}$  asymmetric fission
- Collaboration with JAEA on asymmetric fission of  $^{180}\text{Hg}$  @ JAEA tandem, test of deformed shell ( $Z=38$ ) in GEF code
- Reactor decay heat and anti-neutrino spectra at Jyväskylä
  - $\gamma$  decay gamma strength distribution
  - 15 new nuclei
  - IGISOL + penning trap + JYFLTRAP

#### Planned experiments with detector development

- (n,p) normalization for fission cross section measurements
  - Gas recoil proton detector
  - Precise neutron flux measurement
  - Adapted to work in high neutron density environment
- Conversion electron cross section measurement @ EC-JRC-GELINA
  - DELCO setup
  - CHANDRA product
  - Planned experiment on  $^{238}\text{U}$  in 2018-2019
  - Just set up at GELINA
  - Big challenge is getting higher efficiency
- Reactor decay heat and anti-neutrino spectra at ALTO
  - TAS@ALTO
  - $\beta$ -n emitters
  - exp. planned 2018-2019

#### On-going long term projects

- FIPPS II @ ILL fission fragment mass discrimination and initial kinetic energy PFGS/isotopes as function of FF excitation energy, first exp. planned 2022;
- (n,f) @ nTOF, cross section and angular distributions for Pu and Am, ex. planned, 2021+?
- SOFIA@GSI mass and charge yield, FF kinetic energy and neutrons multiplicity for the U-Pu region using  $^{242}\text{Pu}$  bean 2021+? Big question about cost of cleanup & refurbishment after experiment (1M+ euro). Basically trashes hopes of superheavy research at GSI otherwise;
- Surrogate reaction at storage ring (SUNRISE @ CRYING-FAIR), financial support not secured yet, aim for many actinide targets;
- Innovative TAS with multipurpose detector, but financial support not secured yet.

Much of this work also described in the ND2016 proceedings.

Work aimed at fundamental research.

## 2.7 Comments on AMS measurements for nuclear data, A. Wallner

Recent results using Atomic Mass Spectrometry (AMS), large collaboration. AMS is single atom counting. Several nuclei feasible with  $T_{1/2}$  from 2.7 years.

Typical (?) AMS accelerators: ANU/Canberra, Vienna, ETH Zurich, ANSTO Sydney.

Activation measurement, irradiate then do counting via AMS. Geel, Karlsruhe, Budapest, others.

Irradiation facilities used recently

- keV activations at KIT enabled measurements of  $^{54}\text{Fe}(n,\alpha)$  and many others
- JRC-Geel
- ...

Typical sample size is ~mg, but it is consumed during analysis process. One has to clean up the AMS ion source after each run. That said, cross section extraction quite simple.

If indirect must do post irradiation chemistry before AMS

- $^{238}\text{U}(n,\gamma) \rightarrow ^{239}\text{Np} \rightarrow ^{239}\text{Pu}$  @ IKI, FZK, IRMM
- Th/U @ IRMM, (n,3n), (n,4n), ...

New results

- Irradiate at IRMM, count at ANU
- $^{232}\text{Th}(n,\gamma)^{233}\text{Th}$
- $^{238}\text{U}(n,\gamma)^{239}\text{U}$
- 0.46, 0.52, 1.0, 2.1, 5.0 MeV
- Different from ENDF in both cases, so new work to do

$^{238}\text{U}(n,3n)^{236}\text{U}$

- VERA irradiation
- 17.55, 18.80, 20.05, 22.0 MeV
- Similar measurement at CIAE (Beijing) at 14.2 MeV
- Some scattering in data

$^{232}\text{Th}(n,2n)^{231}\text{Th}$

- 4 different AMS labs to cross check
- 17.55, 18.8, 20.05, 22.0 MeV

Preliminary data on  $^{232}\text{Th}(n,4n+\alpha)^{229}\text{Th}$  (reaction murky)

$^{13}\text{C}(n,\gamma)$  and  $^{14}\text{N}(n,p)$  & AMS of  $^{14}\text{C}$

- Accurate cross section, but wide flux used for irradiation
- PRC publication

$^{54}\text{Fe}(n,\gamma)$

- Vienna (TRIGA) reactor, Budapest reactor for irradiation used to determine thermal point
- Belgia claims Firestone will also have a thermal point for cross comparison

- Also did MACS
- In excellent agreement with ENDF/B-VIII.0 evaluation

$^{54}\text{Fe}(n,2n)$

- Again, in excellent agreement with ENDF/B-VIII.0
- Issue in geometry of irradiation between 2008 and 2010 measurements
- Used Trieste neutron generator for 14.2 MeV points

25 keV irradiations, MACS-like

- AMS seems systematically low compared to other techniques (esp. ToF)
- 7-10% lower
- Fluence measured relative to standards ( $^{197}\text{Au}(n,\gamma)$ )

$^{242}\text{Pu}^{5+}$  vs.  $^{239}\text{Pu}^{5+}$  can easily be distinguished (no isotopic interference). Improvements lead to sensitivity improvement  $\gg 10x$  and reproducibility 2-3% and efficiency  $> 10-100x$ .

## 2.8 Comments on new RPI measurements, Y. Danon

RPI does transmission, capture, fission, etc., capabilities well known. Also, scattering (total neutron production).

Have also used Chi-Nu@LANSE with LANL for  $^{235}\text{U}$  and  $^{239}\text{Pu}$ .

Ta measurements

- Measurements in URR using LSDS, looking now at Ta
- ToF on 45m flight path for capture, transmission just completing
- Therefore will have complete set of new resonances for Ta
- Complete before shut-down

In 2020, will shut down for upgrade. 10x upgrade in fluence.

New detector for neutron scattering in the keV and URR.

Question: Would be useful to investigate Cr & Ni in LSDS. Very useful for benchmarks. Answer: Data in Ph.D. thesis for Ni.

New evaluation of Ag in JEFF

## 2.9 $^{57}\text{Fe}$ neutron inelastic scattering: the interplay between experiment and theory, A. Negret

Recent PRC publication, collaboration between experiment and theorists.

Are measuring  $^{54}\text{Fe}(n,n'\gamma)$  now.

When do  $^{\text{nat}}\text{Fe}(n,n'\gamma)$ , cannot help mix  $^{56}\text{Fe}(n,n'\gamma)$  and  $^{57}\text{Fe}(n,2n'\gamma)$ .

GELINA at EC-JRC at Geel.

GAINS: 12 HPGe detectors + fission chamber ( $^{235}\text{U}$ ) that is used for beam monitoring.



Gamma spectroscopy + neutron ToF, use partial gamma cross sections to back out total inelastic cross section. Of course, it depends on level scheme meaning may find data in conflict with known structure requiring revision of ENSDF level scheme.

1st level in  $^{57}\text{Fe}$  is 14 keV and the emitted gamma is heavily converted with half-life 98.3(3) ns. They kind of made spectroscopy work with Co source, but really did not work so well with  $^{57}\text{Fe}$ . So that transition could not be observed.

Were able to do several other levels/gammas and made comparisons to default EMPIRE and TALYS. Geel != TALYS != EMPIRE != previous ORNL measurements. However, if say EMPIRE could be tuned to match the partial gammas, maybe could determine 14 keV transition and therefore the total (n,inel). M. Sin used an energy dependent tuning to adjust the OM prediction. Some level branchings were also adjusted.

Were able to extract (n,inel) cross section to about 10%, but is more likely a lower bound.

Pronyaev says total non-el cross section cannot be bigger than 1.5 b, why? I guess because it saturates the reaction cross section which is constrained by the optical model.

Big questions about derived shape(s) of  $^{57}\text{Fe}(n,\text{inel})$  extracted. Looking to redo experiment using thinner target & aiming to get that 14 keV transition.

Also did measurement of  $^{16}\text{O}(n,n')$  and  $^{16}\text{O}(p,p')$ , results quite preliminary. Is part of a thesis project.

Structure of  $^{57}\text{Fe}$  is complex as it exhibits shape coexistence

Optical model for odd nuclei is tricky too

## 2.10 JEFF-4, EU projects and JRC involvement, A. Plompen

JEFF-3.3 should be released soon, looking ahead to what can do for JEFF-4.0 (2020-2022 time frame). Aim for writeup for JEFF-3.3 by April.

What's in JEFF-3.3:

- New major actinides “CIELO-2”, collaboration between CEA and IRSN
- TSL data from Cantargi, Granada, Marquez Damian, Noguere (not light water from CAB)
- New decay file from M. Kellett & Bersillon
- New FY file (UKFY3.7)
- Removal of many legacy files
- New covariances, new FY and TSL covariances not in ENDF format yet
- Increased reliance on TENDL
- Improved gamma data and energy balance (C. Jouanne, R. Perry, G. Noguere, O. Serot, ...)
- 8 group structure for delayed neutrons restored (P. Leconte)
- New Cu files (Pereslavitsev, Leal)
- $\gamma, p, d, t, h, a$  from TENDL-2017
- dpa file from KIT

ACTION: need format proposals for:

- TSL covariance
- FPY covariance
- 8 group structure

Looking to process improvements for JEFF-4.0

- Completeness
- Agreed scheme for integrating contributions
- Version and documentation control
- Modern tools for inspection and checking
- Modern tools for benchmarking and validation
- Eliminate limitations (correlated emission? Not viable in ENDF-6 format)

Focus at JEFF has been nuclear energy users, so library not optimal outside that application.

Need accurate data, covariance (to communicate how accurate data is) and best science available.

Cumulative  $\chi^2$  of Mosteller suite is quite good, but are classes of benchmarks where performance is still poor. Particularly for MIXED and INTER cases.

Still many things would like to include in JEFF-4.0 (Neutron Standards, thermal constants, IRDF dosimetry reactions,...). Still discussing with JEFF coordination group.

For  $A > 20$ , TALYS, EMPIRE OK, but below  $A = 20$ , what are the options? R-matrix for sure, also potential models or models based on effective field theory.

Ideally want all projectiles (n, $\gamma$ ,p,d,t,h,a) for fusion, medical, accelerator applications in addition to fission.

Fission yields are another big issue

- Support for evaluation fragile (R.M. Mills)
- New experimental and modeling efforts
- Database & evaluation process not secured
- Alignment with decay data is critical
- Completeness possible with GEF

Decay data equally fragile

- Support for evaluation fragile (M. Kellet)
- Many new experiments
- New data not always used
- again, evaluation process not secured

Masses, structure and decay

- Lacking systematic approach
- Masses: adopt AMDC, but complement with NACRE/Goriely?
- Levels from ENSDF through RIPL
- Consistency with RDD evaluation not automatic nor enforced
- ENSDF evaluations vary in quality and reliability

Thermal neutron scattering

- New experimental data and evaluations
- Covariance information not part of evaluation even though is available
- Issue in solution assemblies with light water

Advocate 2-step approach for JEFF-4.0:

- Evaluation based on microscopic data only, supplemented with TENDL
- Adjustment to integral data to happen later, including not only  $k_{\text{eff}}$

HPRL list has been essential in justifying and therefore acquiring funding for new efforts.

JRC contribution at JEFF:

- Experimental work: Fe
  - $^{54}\text{Fe}(n,n'\gamma)$ ,  $^{56}\text{Fe}(n,n'\gamma)$ ,  $^{54}\text{Fe}(n,n)$ ,  $^{\text{nat}}\text{Fe}(n,n)$
  - Possibly  $^{56}\text{Fe}(n,n'\gamma)$  and  $^{56}\text{Fe}(n,n)$
  - Possibly transmission of Fe vs. thickness
  - $^{54}\text{Fe}$  from ORNL, so careful monitoring activation to avoid 0.6 Bq limit
- Experimental work:  $^{238}\text{U}$ 
  - $(n,\gamma)$  above 100 keV
  - Evaluation process (GMA  $\rightarrow$  covariance)
  - Concern is new highly accurate data not impacting new evaluation enough to make everyone happy
- Experimental work:
  - $^{197}\text{Au}(n,n'\gamma)$  to impact standard?
  - MACS?

In EU, considerable work on minor actinides done, but not integrated into any library. Similarly for FPY & decay.

Need to improve uncertainty on FPY to support long term storage of nuclear waste. “10% is too high”.

## 2.11 Future tools in nuclear data evaluation and envisaged projects at TU Wien, H. Leeb

Focus on light nuclei, esp.  $^{16}\text{O}$  and  $^9\text{Be}$  — both important for fusion applications.

- Methods:
  - Use of statistical models is limited
  - Microscopic models only qualitative
  - Left to work with R-matrix (GECCOS is TU Wien code)
  - Ab-initio approaches
  - Hybrid approaches
- Working on hybrid approach
  - Ph.D. thesis of Benedikt Raab
  - Aim for  $^9\text{Be}$
  - Use R-matrix as calculation tool, supplemented with models

Tools for large scale evaluations up to 250 MeV

- Bayesian statistics
  - Simplified to GLSQR (linearized Bayesian)
  - In GLSQR, limited by dimensionality (too many observables, too many data points, too many grid points)
  - GANDR code has 91k model parameters  $\Rightarrow$  30 Gb for full covariance
  - For modern evaluation, need roughly 1M parameters  $\Rightarrow$  Tb's

- Partial solution is an iterative Bayesian update solution, namely update subspaces of the full covariance matrix and mean value vector using partial sensitivities
  - Neither complete covariance nor evaluation need to be completely stored
  - 3 main steps:
    - Store
      - $s_0$  L, L=# observables
      - $w_i$  N, N=# model calculations
      - U L x N
      - $W_i$  N x N
    - Update
      - M=# data points
    - Reconstruct
  - Benefit in time and size (memory)
  - Demonstrated with TALYS, 2000 calculations, OMP parameters varied: 300 Mb, update in about 15 min on Ta181.
  - To be applied to an evaluated lib. Allows an iterative updating procedure. Assumption: limited exp. correlation.
  - In the future: to be applied to large set of data, many incident particles
- Linear interpolation of all quantities effectively creates a surrogate model for real observables but is preferred because sum rules obeyed easily
- Allows for gigantic problems, but still is reformulation of GLSQR and suffers from all same problems:
  - Model mis-fit/bad model
  - Non-linear response of model on model parameters
  - Lack of sensitivity to model parameter (overly flat response surface)
  - Model parameter degeneracy
  - Unknown-unknowns
  - Correlated experimental data in which correlations are not captured correctly
- Investigating including R-matrix in process

## 2.12 Comments and considerations for CIELO project, Ge Zhigang

For the 1st stage of CIELO:

- Some of the data has been included in different project libraries
- Discrepancies still remain between different CIELO files

Neutron files for future

- Is it needed to do FPY, decay?
- More materials in future collaboration? Current CIELO nowhere near enough for applications
- Important experiments to do?
- Add covariance evaluation as specific topic?

Methodology improvements needed

- Evaluators should take same experimental data or not?
- Models do not agree, can something be done? Which is best?
- Different approaches to covariance generation? Should we recommend specific approach?
- 

Suggestions

- Methodologies and measurement capability must be aligned with current manpower
- Spread evaluation to every material and establish a unique library or continue to focus on few isolated evaluations

- Pay more attention to fundamental theory and experimental studies for both reaction and structure

## 2.13 Nuclear evaluations issues at LLNL, I. Thompson

LLNL is more of a user than a generator, but does make some data.

Specific targets

- $^9\text{Be}$ : well-known performance problems in benchmarking. Also KRUSTY uses BeO (KRUSTY is demo of kilowatt power reactor from NASA for Mars missions).
- $^{233}\text{U}$ : no  $(n,n')$  or  $(n,2n)$  data. No distinctive  $^{232}\text{U}$  gammas to get a handle on  $(n,2n)$ . Also is discussion that need  $(n,\gamma)$  in RRR. Poor performance in critical assemblies. ENDF/B-VIII.0 adopted JENDL-4.0.
- $^{238}\text{Pu}$
- MA
- CP reactions:
  - Needed for NIF diagnostics and material science (ion beam analysis)
  - IBANDL, LANL and LLNL have own too
  - IBANDL at IAEA, but not integrated into an ENDF library
  - Future work should use best practice R-matrix, HF maybe for higher energy/mass
  - IAEA consultant meeting. Planned integration with ENDF and GNDS formats

Classes of reactions

- $(n,n')$ : actinide evaluations often have fake states, typically 2+ and 3- states, used for DWBA to fit data. Is artificial way to change balance between direct and HF. However, predictive power of model decreased as a result. Aiming for Baba data which only exists for  $^{238}\text{U}$ . Dupuis et al (PRC 2011) predicts them from RPM on closed shell nuclei ( $^{90}\text{Zr}$  and  $^{208}\text{Pb}$ ), but work needs to be generalized. Dupuis has now done  $^{238}\text{U}$  as well and it helps.
- $(n,\gamma)$ , primary gammas: need more than just 7-8 nuclei used in ENDF/B-VIII.0
- Delayed fission gamma and neutron emission. ENDF/B only has 6 groups
- Breakup reactions: allow for correlations in breakup products.
  - Especially needed for deuteron-induced reactions.
  - Extend format to triple differential data?
  - Extended R-matrix formalism
  - Hyperspherical harmonic expansions

Need better validated covariances.

## 2.14 Uncertainty estimations for minor actinides, A. Ignatyuk

Problems of systematic uncertainties

- Uncertainties of elastic scattering evaluations for 1H resulted in absurdly small uncertainties <0.2%
- No one believed so dropped back to “expert judgement”

Unrecognized error estimation approach

- Requires data taken with different methods
- MUST TRACK DOWN REFERENCES & DISSECT

Uncertainties for the grand fissiles

- Cross section uncertainties from  $10^{-5}$  -  $10^{-3}$  MeV much, much higher in BROND than standard,
- Russia views standards as unrealistically small for big 3

- Nubar also big differences

#### Role of the criticality benchmarks

- Uncertainty of  $k_{\text{eff}}$  as propagated from evaluations is 10x than benchmark uncertainty, unacceptably high. Is true for all libraries.
- Difficult to take us seriously?

#### Uncertainties on the minor actinides

- Nuclear waste can only realistically be taken care of by burning it in a fast reactor
- For isotope burning, need uncertainties comparable to uncertainties found on major actinides for all minor actinides of interest (like within a factor of 2, not a factor of 10 like now)
- Mainly fission cross section and nubar, but capture cross sections too
- Also, need inelastic scattering on  $^{56}\text{Fe}$ ,  $^{23}\text{Na}$
- $^{241}\text{Pu}(n,f)$  wild difference between Tovesson (2010) and worlds collection of data (mainly from 1970's), below 5 MeV, looks like normalization problem ~factor 3. Maybe bad ToF conversion?
- ENDF/B-VIII.0  $^{241}\text{Pu}(n,f)$  covariance unreasonably small. Evaluation from ORNL in 1988, covariance from LANL in 2010. Nubar covariance wonky too.
- $^{237}\text{Np}(n,f)$  nubar systematically high in ENDF too.  $(n,f)$  cross section in URR has unrealistically low uncertainties.
- $^{241}\text{Am}(n,f)$  cross section has similar issue to  $^{237}\text{Np}$

## 2.15 Nuclear data evaluations at CEA Bruyeres, E. Bauge

### Evaluation methods at Bruyeres...

OMP + sufficiently developed coupled channels to handle direct part of evaluation. Needed to get  $d\sigma/dE$  correct in  $(n,inel)$ . Also must ensure that couple in enough levels to converge fully in direct calculation. It is also important to get the deformation of the levels correct. Use QRPA or similar to determine.

Compound spin distribution impacts pre-equilibrium reaction, too, and not really included in current evaluations.

WFC correction increases elastic and reduces others. GOE vs. Moldauer tests indicate that Moldauer approach is good enough. However, also need Englebrecht-Weidenmueller transform first. So, transform, apply WFC, transform back. This also means have to re-optimize OMP calculation...

Level densities can be constructed via a combinatorial approach. There is a parity asymmetry though in many cases. Impacts  $^{56}\text{Fe}(n,\gamma)^{57}\text{Fe}$ . Spin distribution also important to get right.

Gamma strength functions are normalized to experiment, matching  $\Gamma_\gamma$  and  $D_0$ , is phenomenological, not predictive. Low-level M1 strength helps; removes partial need for normalization. Can the gamma strength function be computed without this at all? QRPA provides a possible solution (Goriely, Peru & Hilaire). CEA has computed these E1 & M1 values for whole table to isotopes. No adjustment needed. Small norm factor still can help a little if want. Will this be generally available? Yes, in RIPL-4. Now also get capture in though the URR, without tweaks. Breaks Brink-Axel assumption, more in line with Oslo results.

Sin et al. PRC 74 (2006) 014608: multi-hump fission barrier. Implemented at CEA. With only class II states cannot reproduce fission, with class III states too can do better, matching data. CEA investigating if can compute barriers with QRPA, rather than by tweaking what is, in say, RIPL. But then must be done consistently with other channels. Barrier heights only need roughly 10% adjustment then.

A microscopic approach means systematic uncertainty estimates within reach because evaluator knobs being removed.

New version of TALYS to be released around this Christmas along with ~350 “best inputs.” Should we consider all microscopic or do parts still need to be handled on a phenomenological basis? Probably some of each.... Gamma ray strength functions are the best candidate for replacing phenomenological approach.

## 2.16 Post-CIELO challenges in actinide evaluations, R. Capote

This is work from the whole CIELO collaboration.

IAEA PFNS CRP will have impact on future evaluations

- $^{235}\text{U}$  PFNS
  - NDS publication
  - Two independent GLSQR fits, mean values in good agreement. These numbers also agree with LANL Madland-Nix fit in NSE
  - Is big difference above 11 MeV (revealed by  $^{90}\text{Zr}(n,2n)$  & other SACS systematics, but it would be really nice to understand the physics behind these systematics)
  - To use this evaluation, must change both nubar and RRR
  - Thermal solution tests show bias vs. ATLF, especially at high leakage. This has been resolved.
  - Including  $(n,\gamma f)$  in nubar in  $^{235}\text{U}$  partially enabled this improvement, although the nubar in  $^{235}\text{U}$  is much rougher than what is in  $^{239}\text{Pu}$
- Similar problem remains for  $^{233}\text{U}$ .  $^{233}\text{U}$  PFNS much harder than  $^{235}\text{U}$
- For  $^{239}\text{Pu}$ , not in bad shape but SG-34 removed the bias already. However, they adjusted PFNS but kept nubar and RRR unchanged. This likely is an issue. SG-34 shows that high leakage solutions are still problematic.
- Propose  $^{233}\text{U}$  and  $^{239}\text{Pu}$  RRR and PFNS

Identified deficiencies in  $^{238}\text{U}$  data

- Q. Sun et al. Fus. Eng. Des. 125 (2017) 9-17
  - ToF, similar to RPI quasi-differential experiment
  - Their conclusion was that JENDL-4.0 was best library
  - CIELO resolves discrepancy at 14 MeV, but added a bigger one around 8-12 MeV
  - Similar result to LLNL Pulsed Sphere findings
  - Similar result to RPI quasi-differential findings
  - At backwards angle, CIELO is still best
- Suspect is problem with  $(n,\text{inel})$  data in CIELO evaluation

Discrepancies in  $^{232}\text{Th}(n,f)$  evaluation/data

- Discrepancies between experiment and all evaluations
- Need to re-evaluate...

## 2.17 CRP on reference database for beta-delayed neutron emission, V. Dimitriou

Aims of the CRP

Compile  $T_{1/2}$ , neutron emission probabilities  $P_n$  and neutron spectra for individual precursors

- $T_{1/2}$ ,  $P_n$  for over 600 precursors

Evaluation existing  $T_{1/2}$ ,  $P_n$  and recommend standards and reference neutron spectra for  $^{235}\text{U}(n_{th})$

- Summation approach
- Using new evaluation, total delayed neutron yield (@ thermal) increases
  - 1.9 -> 2.2 (for ENDF and JENDL), much higher than recommendation
  - 1.6 -> 1.7 (for JEFF) still in line with recommendation, better FPY agreement
- Result of changed decay data, but can see impact of FPY (JEFF in agreement with recommended value, not so much for ENDF or JENDL)
- Recommended values from WPEC/SG-6 in 1999

Need to go back to FPY (IFPY and CFPY) since have largest contribution to uncertainties

- Endorse recommendation for CRP
- Objective: improve existing evaluated FPY
- Participation from Belgium, China, Finland, France, Germany, India, US, Japan, Russia Sweden, UK

Produce systematics and theoretical models to extrapolate to unknown nuclei & recommend new 6 & 8 group constants for delayed nubar for applications

- Piksaikin et al. (Obninsk), made new measurements and produced new systematics
- Previous was WPEC/SG-6
- Many new measurements
- Shown energy dependence
- Developed new systematics
  - new values for  $^{232,233,234,235,236,237,238}\text{U}$
  - $^{234,237}\text{U}$  extrapolation based on these systematics
  - Surprisingly large disagreement between Wilson et al. summation calculation and  $^{235}\text{U}$ . Most likely an issue with the ENDF/B-VII.1 FPY
- Strong energy dependence for  $\langle T_{1/2} \rangle$  for big 3

New group constants and other results will be published in the CRP final report in the Nuclear Data Sheets.

<https://www-nds.iaea.org/beta-delayed-neutron/>

## 2.18 Future fission yield and decay data evaluations, A. Sonzogni

WPEC/SG-25 2005-2008, Assessment of fission product decay data and decay heat calculations, Yoshida, Forrest

- With JEFF, under predict gamma decay heat
- If add TAGS data from Greenwood et al. (INL), improve dramatically prediction of decay heat
- Lead Valencia to study  $^{102,104,105,106,107}\text{Tc}$ ,  $^{105}\text{Mo}$ ,  $^{101}\text{Nb}$ , resulted in PRL
- Another spin-off: improved predictions of anti-neutrino spectra
- Another spin-off: improved understanding of  $\gamma$ -ray emission of neutron unbound states populated in  $\beta$  decay — unusual,  $\gamma$  emission winning over neutron emission. Basically, product has close shell keeping neutrons from being emitted.

In ENDF/B-VI, decay data are old and in bad shape. By ENDF/B-VII.1, situation greatly improved. Further study from BNL enumerated decay products for which the anti-neutrino is highly sensitive. TAGS data have now been included in ENDF decay data.

Fission yields also impact Daya Bay results: anti-neutrino spectra not completely described by FPY and decay data. Is it new physics (more neutrino species) or nuclear data needs work?



Probably ENDF FPY need big help...

NEOS experiment in Korea now also sees unexpected structure in anti-neutrino spectra. This fine structure is a result of application of decay data (individual nuclei contributions to spectrum). With improved FPY, could dramatically improve agreement with NEOS data as well as Data Bay.

Dominant problem isotopes identified:  $^{95}\text{Y}$ ,  $^{98}\text{Nb}$ ,  $^{101}\text{Nb}$ ,  $^{102}\text{Tc}$

On a different note, McCutchan and Kondev noticed that the beta decay used in several medical isotopes is out of date and in poor shape. New measurements have greatly improved this situation and the data included in ENSDF. Neither these improvements nor the CRP results have been included in ENDF/B-VIII.0, but will be for ENDF/B-VIII.1.

Will new FPY get added to ENDF/B-VIII? Nope, not yet.

## 2.19 Present status and future of JENDL, O. Iwamoto

Newest was JENDL-4. Released in 2010, fission products and minor actinides, including covariance

JENDL-4.0u

- Focused on corrections and adding covariances
- 38 files have been updated and are available on the website
- $^{235}\text{U}(n,f)$  covariance was high, its update is much closer to ENDF/B-VIII.0beta3, above 500 keV is JENDL result, below is Leal's result
- New covariance evaluation for Pb isotopes using CCONE and KALMAN, including correlations between multi-order Legendre moments up to order 11. Cannot be processed with NJOY, using in-house code written by O. Iwamoto

JENDL-5.0 in preparation

- Improve reliability of library and completeness
- Revise light nuclei, structural material, FP and actinides
- Include all stable isotopes
- Isomer production for activation
- New R-matrix code AMUR
- New data from J-PARC on minor actinides
- Simultaneous evaluation of fission on all major actinides
- New TSL: mainly water, but others that have hydrogen
- Release planned for 2021, in GNDS?

Light nuclear evaluations

- Using AMUR
- $^{15}\text{N}$  (for ADS)
- $^{16}\text{O}$ ,  $^{19}\text{F}$
- Covariance data

Structural materials

- Want add isomer production data
- Update RP
- $^{93}\text{Nb}$  re-evaluated: A. Ichihara, JNST 53, 2049 (2016)

### Fission products

- Data for light water reactor decommissioning

### Special purpose files

- JENDL decay data files (JENDL/DDF-2015)
- JENDL-4.0 high energy file (JENDL-4.0/HE), up to 200 MeV

### To be released

- JENDL/AD-2017: Activation library
  - Includes  $^{13}\text{C}$  capture cross section, ENDF appears to be missing semi-direct capture component at higher energy
  - $^{63}\text{Cu}(n,\alpha)$
- JENDL/PD-2016: photonuclear library (NEXT WEEK!)
  - Standard version 181
  - Extended version 2000+

## 2.20 Monte Carlo nuclear data adjustment via integral information, D. Rochman

### Assimilation vs. adjustment vs. consistent adjustment

#### Motivation:

- Not all reaction correlations are included in the current evaluations.
- Calculated uncertainties for benchmarks based on current evaluations are large than ICSBEP evaluated uncertainties.
- Some sponsors don't understand and are not happy...

#### Methods for uncertainty reduction

- All methods begin with traditional evaluation to get reasonable Bayesian prior
- Prior parameter pdf determined by looking at what variations are reasonable to bracket EXFOR so correlations between parameters ignored in prior
- Bayesian Monte-Carlo (BMC) == TMC + weights on random files == UMC == Backwards-Forwards MC (BFMC)
  - Generate large number of random files
  - Calculate benchmark for each one
  - Assign weights to realizations  $w \sim \exp(-\chi^2/2)$
  - Update cross section with weights
- Generalized linear least-squares (GLLS) — not discussed, is TSUNAMI way
- Generalized non-linear least-squares (GNLS) == MOCABA + feedback to nuclear data
  - Generate large number of random files
  - Calculate benchmarks
  - Compute sensitivities for each benchmark
  - Not as slow as BMC
  - ANE 77 (2015); JNST paper
- Back to a unique evaluated file?
  - Posterior weights determine best parameters, so just run those
  - Final parameters may not get exactly benchmark number though
    - Test calc with BMC vs. GNLS shows difference in mean between methods
    - Final parameters may not be optimal vs. EXFOR say

- Determines posterior uncertainties/covariances which induce cross material/cross reaction correlations from benchmarks

#### Examples

- Try with HMF1, PMF1, UMF7, MMF3 — Induce correlations between U & Pu
- Tried 12  $k_{\text{eff}}$ , 5 spectral indices
- MCF1 includes U-PU-O, induces correlations between those

We could adjust a library to all benchmarks, but...

- Quality of benchmarks not uniform
- There are many unrecognized correlations in between integral experiments
  - No density measurements done on ORNL parts
  - All LANL crit parts cast with same system
- Many important pieces of information hidden in boxes of archived piles of junk from cleaned out offices

Need sensible requirements for uncertainties on benchmarks, should that be part of our recommendations?

## 2.21 Nuclear data demands for the neutronic design of MYRRHA facility, A. Stankovskiy

### MYRRHA ADS system

- Couples accelerator to reactor
- LBE coolant for operating in subcritical and critical mode
- phase-I 100 MeV accelerator
- phase-II 600 MeV accelerator & couple to reactor

### Data relevant to design & licensing

- Fast neutrons also relevant for Gen-IV reactors, waste burning, ...
- Priority list of isotopes, use sensitivities to  $k_{\text{eff}}$ 
  - $^{239}\text{Pu}$
  - $^{238}\text{U}$
  - $^{240}\text{Pu}$
  - $^{238}\text{Pu}$
  - $^{56}\text{Fe}$
  - Also must pay attention to Pb and Bi isotopes

### VENUS-F zero power facility

- Pb/Bi blocks (simulating LBE fluid, but at room temperature)
- Fast neutron spectrum
- Used for data testing

### Beta\_eff testing

- Preference for JEFF-3.1
- Control rod worth
  - ENDF/B-VII.1 6-group  $^{235}\text{U}$  + JEFF-3.1.2 8-group  $^{238}\text{U}$  untrustworthy, don't mix 6 and 8 group data

### $^{235}\text{U}(n,g)$ fast energies, covariance data

- Bad in ENDF/B-VII.1

- Appears fixed in CIELO

Sodium Fast reactor (ASTRID-like)

- Very large (~100 pcm uncertainty in  $k_{\text{eff}}$ ) due to  $^{238}\text{U}$  inelastic scattering using ENDF/B-VII.1
- With CIELO, hopefully is much reduced

Big-10 (IMF-007)

- Sensitive to URR in fission
- CIELO-1 vs. CIELO-2 comparable
- In CIELO-2: Artificial decrease in  $^{238}\text{U}(n,\gamma)$  compensated by increase in  $^{235}\text{U}(n,\gamma)$

$^{239}\text{Pu}$  testing

- CIELO-1 follows neutron standards, agrees with most experimental data
- CIELO-2 below data

$^{241}\text{Pu}$ :

- Tovesson (2010) data (two different sets taken at LANSE-WNR & Lujan center) significantly lower than all evaluations & all other data
- Desai (2013) only at high energy and agrees with Tovesson

$^{56}\text{Fe}$

- Really sensitive to iron window
- Much happier with CIELO

Pb and Bi

- JENDL-4.0 most reliable below 900 keV
- Highest RRR-URR limit costed to TOF data
- Mihailescu (2008) submitted for possible inclusion in JEFF-3.3
- Production of  $^{210}\text{Po}$  is safety concern, there are quite big differences between libraries, made by  $^{210}\text{Bi}$  beta decay, so  $^{209}\text{Bi}(n,\gamma)$  important. BROND-3.1 has best performance.
- Two campaigns seeking to measure  $^{209}\text{Bi}(n,\gamma)$  in progress

## 2.22 On cross section correlations, uncertainty reduction and calibration from integral data, A. Trkov

Current IAEA CIELO covariances based on measured differential data lead to large uncertainties in criticality benchmarks.

Some correlations are not present in differential data but only appear when internal data included:

- e.g. nubar, fission cross section
- Likely benchmark dependent
- These correlations reduce  $\Delta k_{\text{eff}}$

Play with simplified 1-group toy model.

Initial uncertainty taken from file and uncorrelated.

3 benchmarks considered: Godiva, Big Ten, HISS.

Strong correlation between nubar & fission as implied by Godiva.

Including integral data reduced uncertainty by fact of 2.

Changed mean values, implicit correlations due to this calibration are negligible on HISS benchmark. Only by adding new information (say from new data) can we introduce correlations.

Conclusions from toy model

- Correlations are different for different critical systems
- Correlations are energy dependent
- There exists some similarity between different systems
- Uncertainties on fitted parameters undergo significant reduction when integral data included
- Those uncertainties are insensitive to changes in mean values so no hidden correlations observed

Do we trust critical assembly uncertainties? ORNL cylinders and spheres systematically modeled poorly. The uncertainties should be much larger

## 2.23 Nuclear data and covariance needs for fission reactors and associated fuel cycles, M. Salvatores

Needs assessments:

- SG-26
- Nuclear Data Needs and Capabilities for Applications report

Libraries perform fairly well. Performance can be the result of large compensations which lead to unexpected biases and large uncertainties.  $^{238}\text{U}(n,\text{inel})$  is still a major problem.

Structural and coolant materials still need work (iron, ...).

For optimizing nuclear fuel strategies minor actinides and minor Pu need significant improvements

Covariance data has “holes”, we cannot realistically backfill them all. Covariance High Priority Request List?

Specific needs for novel concepts:

- Molten salt reactors need chlorine,
- Pebble bed reactors need Si and graphite TSL,
- Terrapower traveling wave reactor needs  $^{238}\text{U}(n,\text{inel})$ ,
- ASTRID Na-void reactivity coefficients: needs  $^{23}\text{Na}$  obviously, but really  $^{238}\text{U}(n,\text{inel})$  is bigger problem.

Target accuracy requirements produced in SG-26. Table hasn't been revised in 10 years. An update is needed, product of SG-46?

I would like format extensions to allow more correlations. Also, a finer energy grid should be allowed. Finally, enabling say an eigenvalue decomposition would make Monte-Carlo approaches much easier.

New integral measurements that can help evaluators

- MANTRA irradiations at ATR of small samples of minor actinides for improving capture cross sections
- MASSIMO measurements at NRAD (250 kW TRIGA reactor), oscillation and fission chamber measurements

## 2.24 D. Brown: Future CIELO like activities at BNL

- Isotopes to be looked at because of new data since the last evaluation in mainly ENDF/B:  $^{14}\text{N}$ ,  $^{23}\text{Na}$ ,  $^{27}\text{Al}$ ,  $^{35,37}\text{Cl}$ ,  $^{46,47,48,49,50}\text{Ti}$ ,  $^{50,51}\text{V}$ ,  $^{50,52,53,54}\text{Cr}$ ,  $^{55}\text{Mn}$ ,  $^{58\text{m}1,59}\text{Co}$ ,  $^{58,60,61,62,64}\text{Ni}$ ,  $^{89}\text{Y}$ ,  $^{90,91,92,94,96}\text{Zr}$
- No priority

## 3 TECHNICAL DISCUSSIONS

### 3.1 Lessons learned from CIELO

It is generally agreed that the initial CIELO Pilot Project provided many benefits:

- More efficient use of expertise,
- Experience sharing,
- Wider scrutiny of evaluations (although would have been better to happen earlier),
- More integral testing than we could do ourselves,
- Regular flow of information between projects,
- More visibility and weight:
  - More experiments fielded,
  - Collaboration with EXFOR,
  - Upper management likes it.

### 3.2 General considerations for future CIELO

#### Future strategy

- What are the most important materials left behind by CIELO-1:
  - Need user input
  - HPRL
  - Other user priority lists
  - Should we use what experiments are done to guide us?
  - Should we use sensitivities?
  - Should we use our best judgement?
- Materials correlated with CIELO-1 (Cr, Ni, ...)
- Should we expand CIELO beyond neutron sub-library?

#### Workforce issues

We are stretched very thin, but there are complementary projects that we can (and do) couple to:

- PFNS IAEA project
- R-matrix IAEA project
- Nubar WPEC
- $^{239}\text{Pu}$  RRR WPEC
- Angular distribution WPEC

In fact, the visibility of CIELO helps focus these efforts and helps them justify their efforts.

Everyone wants to keep their in-house evaluation capability. However, there is a real risk that one group's effort will not be accepted by CIELO and hence effort will be wasted. Looks very bad to sponsors. That said, CIELO did inject a lot of energy into the evaluation community.

#### Automation

Also, validation needs to happen continuously, so we always are where we are:

- ADVANCE possibility, but needs automatic benchmarking extension
- NDaST also possibility, only linear response (but is FAST)
- Both need some kind of shared repository (git/svn for ADVANCE, MySQL for NDaST)
- Need to address deep penetration and shielding benchmarks

### Reproducibility

Need to preserve evaluation, so can repeat EVERYTHING: procedures, data, renormalizations, etc. However, it can be an unpopular mandate even though we have TENDL as an example of how it can be realized in practice. With TENDL, a user can “replay” the entire evaluation process. A lower tech scheme is the versioning system used for the CIELO iron evaluation. Here there is enough documentation to redo the evaluation, but the user has to read the comments in the repository carefully. However, neither scheme captures the little decisions entirely that evaluators make during the process. We would need to improve our documentation practices dramatically.

### 3.3 Comments on Fission Product Yields

FPY is recognized as very important. Got report from CRP on beta-delayed-neutrons and indicated that FPY should be future focus.

In the EU, Fission yields and decay data evaluation capability is fragile. The same holds for the US and elsewhere. We should consider collaboration.

ENDF/B-VIII.0 fission product yields are not in good shape.

There will be a separate CRP on fission product yields. So IAEA argues that FPY should not be included in the CIELO project in the future. That said, both US and EU have an interest in new FPY evaluations.

### 3.4 ENDF Format Limitations

Need for cross observable (cross-MF) correlations, e.g. in elastics. There is a way to correlate P0, P1, P2 ..., but we can't process them! For fission, the situation is much worse as so many different quantities are in principal correlated.

ACTION: ENDF-6 need format proposals for:

- TSL covariance
- FPY covariance
- 8 group structure

To support JEFF-3.3 and future ENDF. Or should we just focus on GNDS?

Format extensions to allow more correlations would be welcome. Also, a finer energy grid should be allowed. Finally, enabling, say, an eigenvalue decomposition would make Monte-Carlo approaches much easier.

### 3.5 Many New Experiments

Many new experiments in progress and planned! Too many to list!

- AMS
- Conversion electrons  $\rightarrow$   $^{238}\text{U}(n,n'\gamma)$ , others?
- More Fe
- FPY

## 3.6 Benchmarks and integral adjustment

CIELO-1 depended on differential data but calibrating to integral data means coupling materials and reactions.

There are several ways to do this, and they are generally consistent.

Motivation:

- Not all correlations are included in the current evaluations.
- Calculated uncertainties for benchmarks based on current evaluations are larger than ICSBEP evaluated uncertainties.
- It is well known that, by including integral data, one can reduce data uncertainties. But there are dangers in doing so...
- Some sponsors are trying to reduce design margins and hence cost. So, what can we do to help?

More discussion:

- Correlations are different for different critical systems.
- Correlations are energy dependent.
- There exists some similarity between different systems.
- Uncertainties on fitted parameters undergo significant reduction when integral data are included.
- Uncertainties are insensitive to changes in mean values so no hidden correlations observed.

We could adjust a library to all benchmarks, but...

- Model troubles
  - Models have misfit/don't capture all of physics
  - Models are rigid
- Benchmark troubles
  - Quality of benchmarks not uniform
    - Incomplete specifications (proprietary composition,...)
    - Mistakes
    - Oversimplifications
  - There are many unrecognized correlations in between integral experiments
    - No density measurements done on ORNL parts
    - All LANL critical parts cast with same system
  - Many important pieces of information hidden in boxes of archived piles of junk from cleaned out offices

Need sensible requirements for uncertainties on benchmarks, should that be part of our recommendations?

Breadth in test cases important for full coverage

- Not just critical assemblies...
- Shielding benchmarks played valuable role in e.g. CIELO testing
- Whatever systems adopted for next CIELO, we need a suite of tests for these

When we have bad  $k_{\text{eff}}$ , we actually do not tune the evaluation first — rather we go look for differential data that can inform about what we suspect might be the problem. Data sensitivities as found in NEA's DICE help track down problem data.

Need to educate users of data

- Covariance only includes differential data



- It is OK that mean values are “tuned” to match  $k_{\text{eff}}$  in some cases, but this does not mean we have overestimated uncertainties

New integral measurements that can help evaluators

- MANTRA irradiations at ATR of small samples of minor actinides for improving capture cross sections
- MASSIMO measurements at NRAD (250 kW TRIGA reactor), oscillation and fission chamber measurements

### 3.7 Data deficiencies

#### Inconsistencies

Masses, structure and decay

- Lacking systematic approach
- Masses: adopt AMDC, but complement with NACRE/Goriely?
- Levels from ENSDF through RIPL
- Consistency with RDD evaluation not automatic nor enforced
- ENSDF evaluations vary in quality and reliability

#### Issues in CIELO-1

- $^{56}\text{Fe}$ 
  - resonances
  - (n,inel)
  - Covariances
  - Other parts of steel (Cr, Ni)
- $^{238}\text{U}(n,\text{inel})$
- $^{239}\text{Pu}$ 
  - Nubar
  - PFNS
  - Resonances

#### Issues in ENDF/B-VIII.0

- FPY
- $^{241}\text{Pu}(n,f)$  cross section
- ENDF/B-VIII.0  $^{241}\text{Pu}(n,f)$  covariance unreasonably small. Evaluation from ORNL in 1988, covariance from LANL in 2010. Nubar covariance wonky too.
- $^{237}\text{Np}(n,f)$  nubar systematically high in ENDF too. (n,f) cross section in URR has unrealistically low uncertainties.
- $^{241}\text{Am}(n,f)$  cross section has similar issue to  $^{237}\text{Np}$
- $^9\text{Be}$ : well known performance problems in benchmarking.





**Technical Meeting on  
Long-term International Collaboration to Improve Nuclear  
Data Evaluation and Evaluated Data Files**

IAEA Headquarters, Vienna, Austria  
18-21 December 2017  
Meeting Room VIC C0343

### Adopted Agenda

#### Monday, 18 December

**08:30 – 09:30**    **Registration** (IAEA Registration desk, Gate 1)

**09:30 - 10:00**    **Opening Session**

Welcoming address – Arjan Koning, SH-NDS  
Introduction – R. Capote, NDDU/NDS  
Election of Chairman and Rapporteur  
Adoption of Agenda  
Administrative matters

**10:00 - 13:00**    **Presentations by participants** (~30 min /~7 min discussion each)

1. *CIELO iron evaluation - lessons learned and vision of CIELO's future*, M.W. Herman
2. *Benchmarking of the latest Neutron and Gamma Transport Cross Sections for Oxygen, Iron and Uranium in the clean Benchmarks driven by D-T and <sup>252</sup>Cf sources*, S. Simakov

*Coffee breaks as needed in between*

**13:00 – 14:30**    **Lunch**

**14:30 – 18:00**    **Presentations by participants (cont'd)**

*(remote) Comments on CIELO project and future work*, M.B. Chadwick

3. *Possible improvements in the neutron cross section evaluation*, V.G. Pronyaev
4. *Lessons learned from CIELO evaluations and experimental needs*, R. Capote

*Coffee breaks as needed in between*

#### Tuesday, 19 December

**09:00 - 13:00**    **Presentations by participants (cont'd)**

1. *Foreseen experimental activities at CNRS-IN2P3 related to nuclear energy researches (2018-2021 and beyond)*, M. Kerveno
2. *Comments on AMS measurements for nuclear data*, A. Wallner
3. *Comments on new RPI measurements*, Y. Danon
4. *<sup>57</sup>Fe neutron inelastic scattering: The interplay between experiment and theory*, A. Negret
5. *JEFF-4, EU projects and JRC involvement*, A.J. Plompen

**13:00 – 14:00**    **Lunch**

**14:00 – 18:00**    **Presentations by participants (cont'd) & Round table discussion**

6. *Comments and consideration for CIELO project*, Ge Zhigang
7. *Nuclear Evaluation Issues at LLNL*, I. Thompson
8. *Uncertainty estimations for minor actinides*, A.V. Ignatyuk
9. *Nuclear Data evaluations at CEA Bruyeres*, E. Bauge
10. *Challenges in actinide evaluations*, R. Capote
11. *Future fission yield and decay data evaluations*, A. Sonzogni and P. Dimitriou

**Discussions on evaluation methodology and planned evaluations**

*Coffee breaks as needed in between*

**Wednesday, 20 December**

**09:00 - 13:00**    **Presentations by participants (cont'd) & Round table discussion**

1. *Monte Carlo Nuclear Data Adjustment via integral information*, D. Rochman
2. *Nuclear data demands for the neutronic design of MYRRHA facility*, A. Stankovsky
3. *On Cross Section Correlations, Uncertainty Reduction and Calibration from Integral Data*, A. Trkov
4. *Nuclear data and covariance needs for fission reactors and associated fuel cycles: an update*, M. Salvatores

**Further discussions on planned evaluations and measurements**

**13:00 – 14:00**    **Lunch**

**14:00 – 17:30**    **Round table discussion (cont'd)**

**Drafting of the Summary Report including Recommendations and Action List**

*Coffee breaks as needed in between*

**19:00**            **Dinner at a restaurant (see separate information sheet)**

**Thursday, 21 December**

**09:30 - 12:00**    **Drafting of the Summary Report including Recommendations and Action List (cont'd)**

**12:00**            **Closing of the meeting**

*Coffee break as needed in between*

**Technical Meeting on  
Long-term International Collaboration to  
Improve Nuclear Data Evaluation and Evaluated Data Files**

18 to 21 December 2017

IAEA, Vienna

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## ANNEX 3

### Presentations

#	Author	Title	Link
1	M.W. Herman	CIELO iron evaluation - lessons learned and vision of CIELO future	<a href="#">PDF</a>
2	S. Simakov	Benchmarking of the latest Neutron and Gamma Transport Cross Sections for Oxygen, Iron and Uranium in the clean Benchmarks driven by D-T and Cf-252 sources	<a href="#">PDF</a>
3	M.B. Chadwick	Comments on CIELO project and future work	--
4	V.G. Pronyaev	Possible improvements in the neutron cross section evaluation	<a href="#">PDF</a>
5	R. Capote	Lessons learned from recent evaluations and experimental needs	<a href="#">PPTX</a>
6	M. Kerveno	Foreseen experimental activities at CNRS-IN2P3 related to nuclear energy researches (2018-2021 and beyond)	<a href="#">PDF</a>
7	A. Wallner	Recent AMS measurements on neutron-induced reactions + outlook	<a href="#">PPTX</a>
8	Y. Danon	Comments on new RPI measurements	--
9	A. Negret	Fe-57 neutron inelastic scattering: The interplay between experiment and theory	<a href="#">PPTX</a>
10	A.J. Plompen	JEFF-4, EU projects and JRC involvement	<a href="#">PPTX</a>
11	D. Brown	Future CIELO activities at BNL	<a href="#">PDF</a>
12	Ge Zhigang	Comments and consideration for CIELO project	<a href="#">PPT</a>
13	I. Thompson	Nuclear Evaluation Issues at LLNL	<a href="#">PPTX</a>
14	A.V. Ignatyuk	Uncertainties for minor actinides	<a href="#">PPT</a>
15	E. Bauge	Improving reaction modeling	<a href="#">PPTX</a>
16	R. Capote	Post-CIELO challenges in actinide evaluations	<a href="#">PPTX</a>
17	A. Sonzogni	Some of the progress made since WPEC SG 25,	<a href="#">PPTX</a>
18	P. Dimitriou	Recommendations from IAEA CRP on beta-delayed neutron emission	<a href="#">PPTX</a>
19	O. Iwamoto	Plans for JENDL-5 evaluations	--
20	H. Leeb	4. Future Tools in Nuclear Data Evaluation and Envisaged Projects at TU Wien	<a href="#">PPTX</a>
21	D. Rochmann	Monte Carlo Nuclear Data Adjustment via integral information	<a href="#">PDF</a>
22	A. Stankovskiy	Nuclear data demands for the neutronic design of MYRRHA facility	<a href="#">PDF</a>
23	A. Trkov	On Cross Section Correlations, Uncertainty Reduction and Calibration from Integral Data	<a href="#">PPTX</a>
24	M. Salvatores	Nuclear data and covariance needs for fission reactors and associated fuel cycles: an update	<a href="#">PP</a>





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