IAEA
International Atomic Energy Agency
Atoms for Peace and Development

IAEA Nuclear Data Section: On-going and future Data Development Projects (DDPs)

Roberto Capote
Deputy Section Head, NDDU head

33th Meeting of International Nuclear Data Committee, March 2021, IAEA, Vienna

Data Development Projects

1.- Maintain the international Neutron Standards file and evaluation techniques (NDS staff, SSAs, TM/CM, CVs, DT)

Neutron Data Standards webpage: https://nds.iaea.org/standards

- CM on "Neutron Data Standards" (virtual), Vienna, Austria, 12-16 October 2020

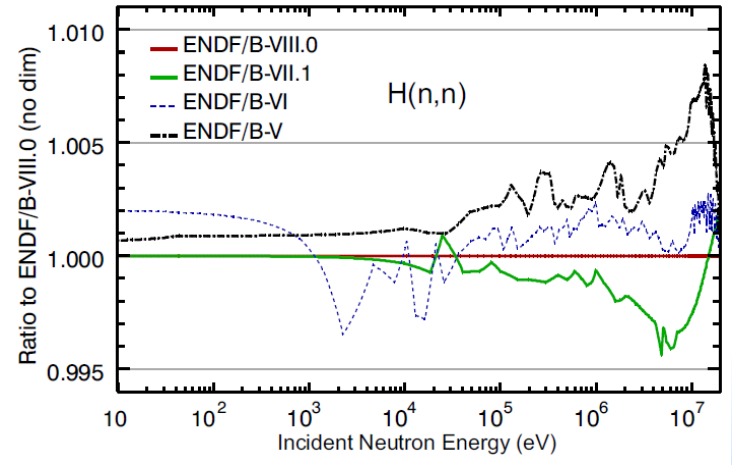
✓ modernization of GMA code - conversion to Python (G. Schnabel)
https://github.com/IAEA-NDS/DATP-Python

✓ Nucl. Data Sheets **163** (2020) 280-281

Corrigendum to: "Evaluation of the Neutron Data Standards" [Nucl. Data Sheets 148, p. 143 (2018)]

A.D. Carlson,[1,*] V.G. Pronyaev,[2] R. Capote,[3] G.M. Hale,[4] Z.-P. Chen,[5] I. Duran,[6] F.-J. Hambsch,[7] S. Kunieda,[8] W. Mannhart,[9,†] B. Marcinkevicius,[3,10] R.O. Nelson,[4] D. Neudecker,[4] G. Noguere,[11] M. Paris,[4] S.P. Simakov,[12] P. Schillebeeckx,[7] D.L. Smith,[13] X. Tao,[14] A. Trkov,[3] A. Wallner,[15,16] and W. Wang[14]

✓ Nucl. Data Sheets **148** (2018) 143-188



VI. CONCLUSION AND OUTLOOK

Results have been obtained for the nuclear data standards in this investigation. Concerns about the rather small uncertainties obtained for the standards in previous evaluations, led us to investigate one aspect of unknown systematic uncertainties. We realize that in some cases our previous uncertainties had been underestimated. The larger uncertainties now obtained result from unknown systematic uncertainties based on the spread in normalization factors of absolute measurements for each cross section type. Also improved determinations of the uncer-

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- ^{1}H(n,n) : 0.34%
- ^{6}Li(n,t) : 0.5%
- C(n,n) : 0.8%
- ^{10}B(n,α) : 0.5%

- ^{197}Au(n,γ) : 1.7%
- ^{238}U(n,γ) : 1.7-2.4%
- ^{235}U(n,f) : 1.2%

valid for all actinides measured with fission chambers

- ^{252}Cf(s.f.) ν_{tot} : 0.4%

valid for all actinides

RC & D. Neudecker
arXiv 1908.00272 (2019)
Energy dependence forces reevaluation

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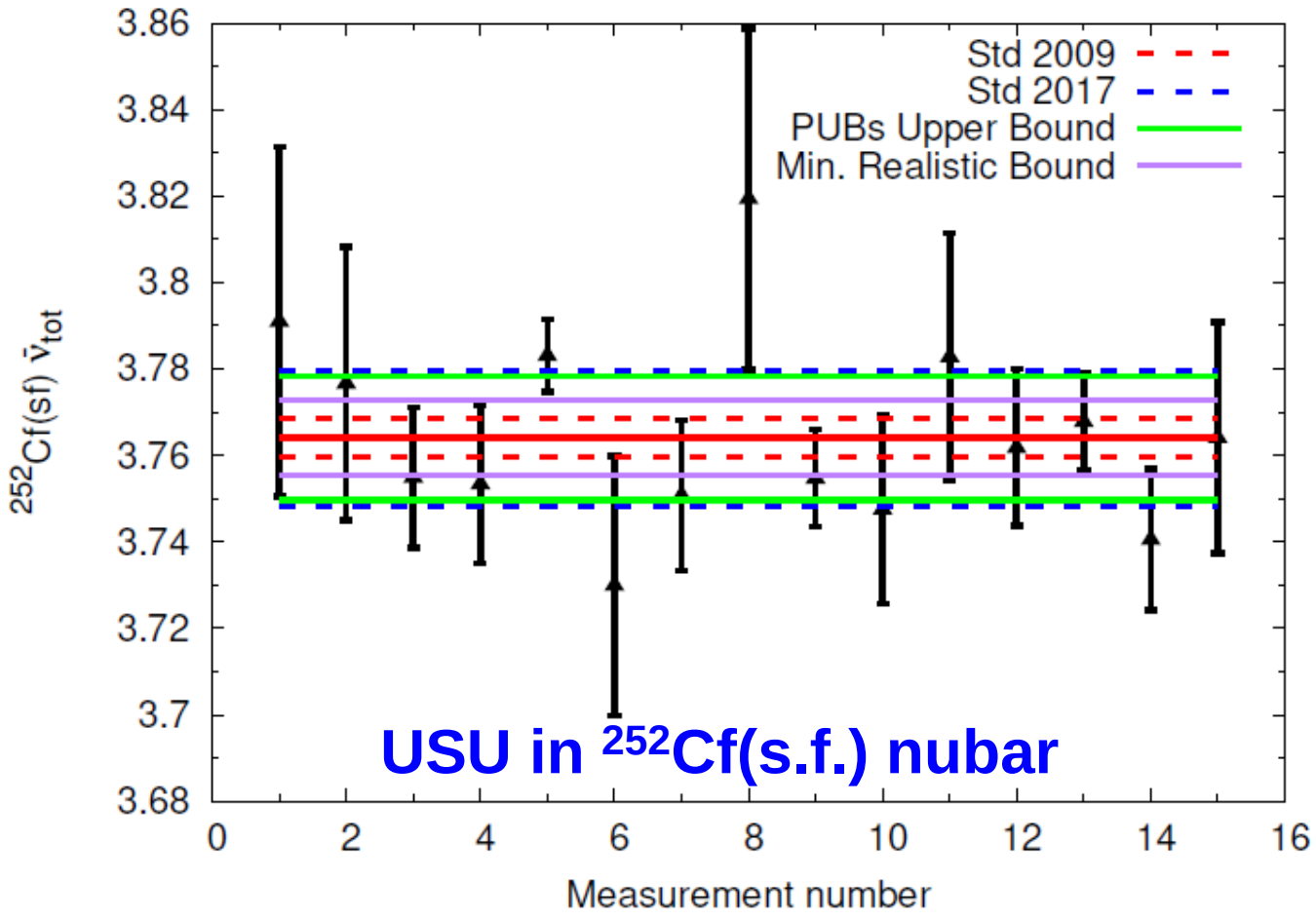

Std 2009:
0.13%
(too small)

Std 2017:
0.42%
(slightly large?)

PUB upper:
0.38%
PUB min. real.:
0.23%

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1.- Maintain the international Neutron Standards file and evaluation techniques (NDS staff, SSAs, TM/CM, CVs, DT)

Participants of the CM on UQ

Three CMs:
3-6 Dec. 2018
6-10 May 2019
July 2020

RC et al, Nucl. Data Sheets **163** (2020) 191-227

Unrecognized Sources of Uncertainties (*USU*) in Experimental Nuclear Data

R. Capote,[1,*] S. Badikov,[2] A. Carlson,[3] I. Duran,[4] F. Gunsing,[5] D. Neudecker,[6] V.G. Pronyaev,[7] P. Schillebeeckx,[8] G. Schnabel,[9] D.L. Smith,[10] and A. Wallner[11]

[1] *NAPC–Nuclear Data Section, International Atomic Energy Agency, A-1400 Vienna, Austria*
[2] *Atomstandard, Rosatom State Corporation, Moscow, Russia*
[3] *National Institute of Standards and Technology, Gaithersburg, MD 20899, USA*
[4] *Universidade de Santiago de Compostella, 15782 Santiago de Compostela, La Coruna, Spain*
[5] *CEA Irfu, University Paris-Saclay, F-91191 Gif-sur-Yvette, France*
[6] *Los Alamos National Laboratory, Los Alamos, NM 87545, USA*
[7] *Contractor, NAPC–Nuclear Data Section, International Atomic Energy Agency, A-1400 Vienna, Austria*
[8] *Joint Research Centre - Geel, 2440 Geel, Belgium*
[9] *Uppsala University, Lagerhyddsvagen, 75120 Uppsala, Sweden*
[10] *Argonne National Laboratory, 1710 Avenida del Mundo, No. 1506, Coronado, CA 92118, USA*
[11] *Australian National University, Canberra ACT, Australia*

(Received 9 August 2019)

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2.- Nuclear Data for Ion Beam Analysis applications (NDS staff, CVs, SSA)

- **The IBANDL webpage** has been maintained and extended (see www-nds.iaea.org/exfor/ibandl.htm).
- P. Dimitriou, V. Semkova (SSA) and V. Zerkin are important contributors.
- R-matrix evaluations are being developed (see R-matrix codes and INDEN)

3. Charged-Particle Monitor Reactions and Nuclear Data for Medical Isotope Production, 2019-2023 (NDS staff, 4 SSAs/year)

- A. Hermanne, F. T. Tárkányi, A. V. Ignatyuk, , S. Takacs, R. C. **(20 reactions)**
  Upgrade of IAEA recommended data of selected nuclear reactions for production of PET and SPECT isotopes, under review NDS, April 2021
  arxiV-2006.03125(2020)

- A. Hermanne, F. T. Tárkányi, A. V. Ignatyuk, , S. Takacs, R. C. **(25 reactions)**
  Upgrade of recommended nuclear cross section data base for production of therapeutic radionuclides, to be submitted to JRNC (June 2021)

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4.- R-matrix codes for Charged-Particle Reactions in the Resolved- Resonance Region (CVs, NDS staff, DT)

Three CMs held in 2015, 2016, and 2017.

4th CM on 27-29 August 2018:

– Inter-comparison of R-matrix codes and preparation of publication (AMUR, AZURE, CONRAD, EDA, GECCCOS, SAMMY, SFRESCO)
After a rough start now all codes agree within 1-2%

– **Publication: Thompson et al., Eur. Phys. Jour. A 55, 72 (2019)**

5th CM on 13-14 May 2019:

– Test 2: inter-comparison of minimization techniques and calculation of covariances by different codes (AZURE, CONRAD, EDA, SAMMY, SFRESCO)

– Test 3: full evaluation of ^{7}Be system produced by: ^{3}He+^{4}He, p+^{6}Li

– **Results of global fitting of ^{7}Be with RAC: INDC(NDS)-0791**

Also important for INDEN: evaluations of light elements

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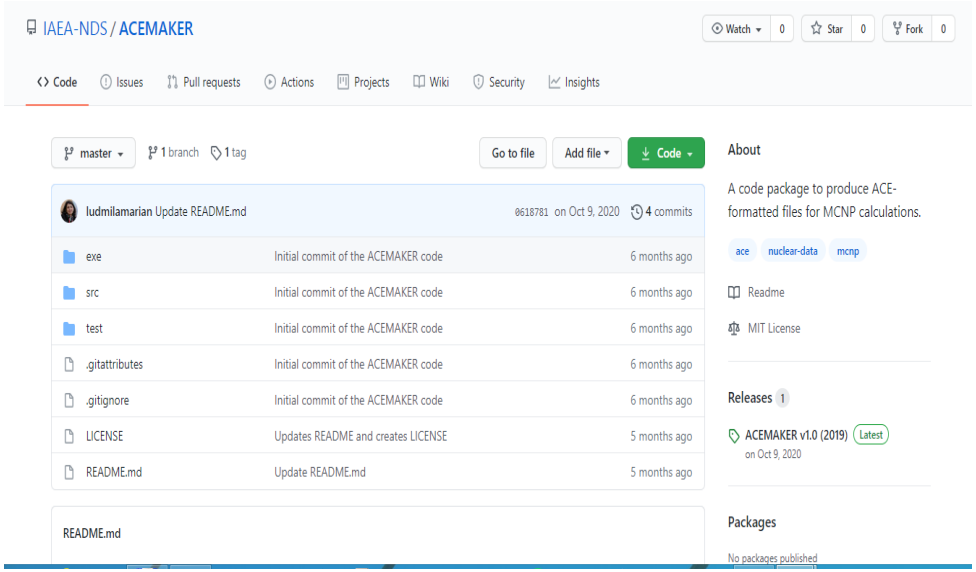
5.- ACEMAKER: Package to produce ACE-formatted files for MC calculations based on PREPRO (SSAs, NDS staff, CVs)

Current capabilities

- Based on PREPRO (2019) pre-processing package by D. E. Cullen
- Intermediate files in ENDF-6 format
- Prepares ACE-formatted file for incident neutrons for MC transport

https://github.com/IAEA-NDS/ACEMAKER



Current developments and V&V in progress

- Thermal scattering law preparation
- Dosimetry reaction files
- Charged-particle production

- **Open source github-based dissemination based on PREPRO**
- **An alternative for independent IAEA ND processing and evaluation, which also serves as a benchmarking/validation tool**

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6.- Stopping Power Database (1 SSA, CV, NDS staff)

www-nds.iaea.org/stopping/

The compilation of experimental electronic stopping powers that was created and maintained for decades by Prof. Helmut Paul, Univ. Linz, has been passed over to IAEA NDS in December 2015. Claudia Montanari, an external consultant is being funded through SSAs to maintain and extend the Stopping Power database in collaboration with P. Dimitriou and L. Mariam (web design).

7.- Gamma-production data for capture and inelastic scattering (SSA, CV, DT, NDS staff)

- Evaluation of Thermal Neutron Capture Gamma Spectra, **INDC(NDS)-0810** Developments of the evaluation pipeline and benchmarking data are required.
- Additional needs and/or evaluated data deficiencies have been identified (geology, space applications, forensic, security, etc).
- NDS developed and maintain PGAA and EGAF databases that may require updating.

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8. Decay Data for Monitoring Applications, 2019-2022 (3 SSAs/year, RC, CMs)

Objective:

to create a library of decay data for radionuclides relevant to the Comprehensive Test-Ban-Treaty Organization Preparatory Commission (CTBTO)

- Duration: 2019 – 2022 (2023?)
- Product: online decay data library
- Output: publication in peer-reviewed journal

Participants

Jun Chen, NSCL, MSU

Tibor Kibedi, Australian National University

Filip Kondev, Argonne National Laboratory *(Technical Coordinator)*

Alan Nichols, Surrey University

Alexander Negret, IFIN-HH

Sorin Pascu, IFIN-HH

Balraj Singh, McMaster University

Jagdish Tuli, University of Berkeley

Meetings

- Kick-off meeting: IAEA, 6-8 May 2019
- 1st Virtual Meeting: 12 May 2020
- 2nd Virtual Meeting: 25-27 Aug. 2020
- 3rd Virtual Meeting: 16 November 2020
- 4th Virtual Meeting: 17 December 2020
- 2nd IAEA TM (virtual), 24-26 March 2021

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8. Decay Data for Monitoring Applications, 2019-2022 (3 SSAs/year, RC, CMs)

Participants of the Decay Data CM

Priority nuclides

Radionuclides	Half-Life	Decay mode
Zr-95	64 d	B-
Nb-95	35 d	B-
Zr-97	17 h	B-
Mo-99	66 h	B-
Ru-103	39 1/4 d	B-
Rh-105	35 1/3 h	B-
Ru-106	373 3/5 d	B-
Cd-115m	44 3/5 d	B-,IT
Cd-115	53 1/2 h	B-
Sb-126	12 1/2 d	B-
Sb-127	3 6/7 d	B-
Te-131m	30 h	B-,IT
I-131	8 d	B-
I-133	20 4/5 h	B-
Xe-133	d	B-
Xe-133m	d	B-
Xe-135	h	B-
Te-132	3 1/5 d	B-
Cs-136	13 1/6 d	B-
Cs-137	30 y	B-
Ba-140	12 3/4 d	B-
La-140	1 2/3 d	B-
Ce-139	d	EC
Ce-141	32 1/2 d	B-
Ce-143	33 h	B-
Ce-144	284 8/9 d	B-
Nd-147	11 d	B-
Nb-97	72.1 m	B-
Rh-106	30.07 s	B-
Te-127	9.35 h	B-
I-132	2.295 h	B-
Pr-143	13.57 d	B-
Pr-144	17.28 m	B-

Data needs:

42 fission products

42 activation products

Xe isotopes (noble gas detection)

Top Priority:
30 fission products + 3 Xe isotopes

Status:

Half of the evaluations completed

Reviews underway

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9. Nuclear Data for Decay Heat, anti-neutrino spectra, and other applications (SSA, TM/CM, NDS staff)

1) CM, 19-21 February 2018

Participants
Alejandro Algora
Muriel Fallot
Filip Kondev
Gopal Mukherjee
Alan Nichols
Krzysztof Rykaczewski
Alejandro Sonzogni
Jose-Luis Tain
Tadashi Yoshida

Scientific Secretary
P. Dimitriou

Consultant's Meeting on Updating Data Needs for Total Absorption Gamma-ray Spectroscopy (TAGS)

19-21 February 2018, IAEA Headquarters, Vienna, Austria

Objective

The objective of the meeting is to review the current state of affairs regarding TAGS facilities & measurements, TAGS data and decay data libraries, impact of new TAGS data on decay heat calculations, anti-neutrino spectra,etc, discuss new emerging data needs and make recommendations for the future.

Presentations and discussions will focus on the following items:

Presentations: nds.iaea.org/index-meeting-crp/TAGS2018/

Following meeting recommendations: **DDP on current decay data needs and impact of new TAGS measurements on decay heat and anti-neutrino spectra calculations**

Purpose: assess available nuclear structure and decay data of fission products with major contribution to decay heat, and anti-neutrino spectra and recommend new measurements (TAGS, high-resolution gamma-spectroscopy), and new evaluations:

- ✓ Decay data of 114 important fission product yields assessed by: Nichols (SSA), Algora, Kondev, Yoshida
- ✓ Compilation of new mean beta and gamma energies using latest available TAGS data: Dimitriou
- Calculations of decay heat for major actinides and anti-neutrino spectra using recent TAGS measurements to assess impact: Fallot, Sonzogni, Yoshida
- Publish results: preparation of paper in progress (Dimitriou, Nichols, et al.)

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9. Nuclear Data for Decay Heat, anti-neutrino spectra, and other applications

2) TM, 23-26 April 2019

- 36 participants from 10 countries
- Report INDC(NDS)-0786
- Recommendations for anti-neutrino spectra experiments and data analysis, decay data and reactor data
- Objectives:
  - assess the sensitivity of the observations to uncertainties affecting large and short-baseline anti-neutrino measurements
  - address the limitations and uncertainties of the theoretical methods (conversion vs summation)
  - estimate their dependence on the available data (beta spectra, decay data, fission yields)
  - make recommendations for the existing measurements, theories and evaluations and
  - new proposals for the future where needed, stimulate cross-collaborations
- Follow-up TM planned

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10.- Decay and reaction data for the back-end of the fuel cycle: monitoring, characterization, decommissioning , and disposal of spent-fuel and other irradiated materials (NDS staff, TMs/CMs, DTs, CVs, SSAs)

CM organized on 2-4 November 2020, IAEA, Vienna (virtual)

- XS & DD for NPP decommissioning and waste transmutation
  - LLFP transmutation and activation XS for decommissioning
  - UQ is critical to identify potential problems in waste storage
  - High-energy neutron and proton induced reaction data up to 200 MeV
- ND for fusion waste management: decay and reaction data including
  - Activation/transmutation rates for 10-16 MeV neutrons in structural materials (e.g., W, Mo, Fe, Ni, Cr, Mn, C, Nb). Data of minor isotopes important !
  - UQ is critical as impurities (e.g., uranium in Be, Co in W) may hinder the processing of waste and induce radiological hazards
  - Gas production cross sections

11.- Decay and reaction data for neutron production: the (α,n) reactions (NDS staff, TMs/CMs, DTs, CVs, SSAs)

1 day CM organized in March 2021 within INDEN-LE, IAEA, Vienna (virtual)

- **(α,n)** reactions and SF are the main neutron term in spent fuel, follow-up planned.

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12.- Development of evaluation methodology and nuclear reaction modelling systems (NDS staff, CMs, DTs, CVs, SSAs)

- Evaluation Pipeline prototype, G. Schnabel, arxiv.org/abs/2009.00521
- Prototype of EXFOR JSON CouchDB database https://github.com/IAEA-NDS/exfor-couchdb-docker
- Prototype website showing a version tracking workflow for libraries https://www-nds.iaea.org/index-meeting-crp/CM-FENDL-2020-11/docs/2020-11-23%20FENDL%20-%20Georg%20Schnabel.pdf
- Prototype of an AI/ML approach to find Exforable papers www.gschnabel.com/storage/posters/202008_MLSS_Skoltech_poster_Georg_Schnabel.pdf

- **EMPIRE, TALYS and GANDR code development**
  - Additional work on code development and testing, evaluation backbone of ALL.
  - GANDR-5.3 released in 2019, GANDR GUI developed by J. Malec (SSA)
  - TALYS new version released (see more information in Koning (other)

- **Many technical papers published on EMPIRE and TALYS applications**


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Thank you!