https://doi.org/10.61092/iaea.hs75-523t

INDC(NDS)-0654
Distr. G+NM

IAEA
International Atomic Energy Agency

INDC International Nuclear Data Committee

Summary Report

Consultants' Meeting on

Recommended Input Parameters for Fission Cross-Section Calculations

IAEA Headquarters
Vienna, Austria
17 – 18 December 2013

Roberto Capote Noy, IAEA, Vienna, Austria
Stephane Goriely, ULB, Belgium
Stephane Hilaire, CEA, France
Osamu Iwamoto, JAEA, Japan
Toshihiko Kawano, LANL, USA
Arjan Koning, NRG, The Netherlands
Stanislav Simakov, IAEA, Vienna, Austria

December 2014

IAEA Nuclear Data Section
Vienna International Centre, P.O. Box 100, 1400 Vienna, Austria

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Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre
PO Box 100
1400 Vienna
Austria

Printed by the IAEA in Austria

February 2015

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Toshihiko Kawano, LANL, USA
Arjan Koning, NRG, The Netherlands
Stanislav Simakov, IAEA, Vienna, Austria

Abstract

A Consultants' Meeting on "Recommended Input Parameters for Fission Cross-Section Calculations" was held at IAEA Headquarters, Vienna, Austria to define the scope, deliverables and appropriate work programme of a possible Coordinated Research Project (CRP) on the subject. Presentations are available online at https://www-nds.iaea.org/index-meeting-crp/CM-RIPL-fission/. A new CRP was endorsed to recommend a comprehensive set of fission input parameters needed for the modelling of fission cross sections. Special attention will be given to the modelling of photon and nucleon induced reactions on actinides with emphasis on incident energies below 30 MeV. The goals and detailed deliverables of the planned CRP were proposed. A Hauser-Feshbach code intercomparison was recommended.

December 2014

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1. INTRODUCTION

Nuclear data for energy applications continue to be of considerable interest to the IAEA. Reliable safety cases require predictions of key performance parameters of reactor systems and the fuel cycle with credible values and uncertainty estimates. Sensitivity analyses for GenIII+, GenIV and Accelerator Driven Systems further show that target uncertainties for certain nuclear data have to be very tight. This certainly applies to capture, fission and inelastic scattering cross sections of the major actinides: ^{232}Th, ^{233,235,238}U, and ^{239}Pu. It is therefore mandatory to provide nuclear data to the required accuracies together with reliable uncertainties.

While experimental data provide extremely important constraints for evaluated data, it is well established that nuclear modelling is required to fill the gaps in data and make evaluated data files both complete and physically consistent. The difficulty is that practical use of nuclear theory and models in supplying nuclear data for applications requires considerable input of model parameter data and nuclear constants. Therefore the International Atomic Energy Agency (IAEA) has worked extensively since 1993 on a library of validated nuclear-model input parameters, referred to as the Reference Input Parameter Library (RIPL). The third RIPL coordinated research project (RIPL-3) was brought to a successful conclusion in December 2008, after 15 years of challenging work carried out through three consecutive IAEA projects. The RIPL-3 library was released in January 2009, and is available on the Web through http://www-nds.iaea.org/RIPL-3/, and a comprehensive technical paper describing the contents of the IAEA Reference Input Parameter Library was published[1].

The RIPL data and methodology in the derivation of evaluated nuclear reaction data have been adopted by major national evaluation projects worldwide, and used in the derivation of ENDF/B-VII.0, ENDF/B-VII.1, JENDL-4, CENDL-3.1 and JEFF-3.2 nuclear applications libraries. The RIPL database is also very valuable to theoreticians involved in the development and use of nuclear reaction modelling (e.g. CoH3, CCONE, EMPIRE, GNASH, UNF, and TALYS) both for theoretical research and nuclear data evaluations.

The improved quality of the input parameters made nuclear reaction modelling much easier, reproducible and robust, and also enhanced the use of reaction modelling in nuclear data evaluation. However, some problems have been identified since the latest RIPL database release, in particular, RIPL input parameters for fission have not been comprehensively validated against available experimental data, and therefore do not guarantee a reproducible and/or accurate calculation of fission cross sections. A large variability in calculated fission cross sections is observed due to the use of different fission formalisms, implementation in the codes, and/or combination of parameters. To address those data needs an IAEA Consultants' Meeting on *Recommended Input Parameters for Fission Cross-Section Calculations* has been organized. Five consultants attended the meeting. S. Goriely agreed to act as rapporteur. The IAEA was represented by S. Simakov, P. Dimitriou, M. Verpelli and R. Capote, who served as Scientific Secretary. The approved Agenda is attached (Appendix 1), as well as a list of participants and their affiliations (Appendix 2), and the meeting photo

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[1] R. Capote, M. Herman, P. Oblozinsky, P.G. Young, S. Goriely, T. Belgya, A.V. Ignatyuk, A.J. Koning, S. Hilaire, V.A. Plujko, M. Avrigeanu, O. Bersillon, M.B. Chadwick, T. Fukahori, Zhigang Ge, Yinlu Han, S. Kailas, J. Kopecky, V.M. Maslov, G. Reffo, M. Sin, E.Sh. Soukhovitskii, and P. Talou, RIPL – Reference Input Parameter Library for Calculation of Nuclear Reactions and Nuclear Data Evaluations, *Nucl. Data Sheets* **110** (2009) 3107–3214

(Appendix 3). R. Capote welcomed the participants, and emphasized the significance of their role in updating the RIPL database and defining the scope and programme of work for a successful CRP if recommended. A summary of the meeting is given below. Presentations are available online at https://www-nds.iaea.org/index-meeting-crp/CM-RIPL-fission/.

2. MEETING SUMMARY

Charge to the Consultants

The charge to the Consultants included assessment of the need for a new CRP and to define its scope and the deliverables and propose possible participants. The focus of a new CRP will be on input parameters for fission cross-section calculations, but a comprehensive update of other RIPL Segments could be included if resources allow.

General outcome

The Consultants determined that there exist grounds for a new Coordinate Research Project by the IAEA. RIPL database has become 'de-facto' reference for input parameters used in nuclear reaction modelling; however, there are additional needs and/or deficiencies identified in the fission input parameters that require further work. There are also additional updates needed in other RIPL Segments (e.g. masses, levels, etc.).

Scope of the new CRP

Recommend a comprehensive set of input parameters with estimates of uncertainties needed for modelling of fission cross sections based on microscopic and phenomenological approaches. Priorities will be given to the modelling of photon and nucleon induced reactions on actinides and a description of relevant reaction channels with emphasis on incident energies below 30 MeV.

Model input parameters to be considered

Fission parameters

Input parameters will be provided according to the following three descriptions of the fission path: fission barriers (parabolic), barrier and wells (parabolic), full 1D fission path (as in RIPL-3)

- Compilation of available sets of empirical fission barriers (heights and widths) used in reaction calculations
- Compilation of available sets of class II/III states in the well(s) for accurate prediction of near threshold resonances
- Compilation of available sets of transition states and tabulated level densities at the saddle points, and corresponding tabulated ground state level densities.
- Compilation of available sets of theoretical barriers (including symmetries) and comparison with recommended empirical set to assess the predictive power

Other input parameters

- Compilation of available sets of optical model potentials for actinides
- Compilation of available sets of gamma-ray strength functions for actinides
- Compilation of available sets of theoretical masses and ground state deformations
- Update of sets of discrete levels and decay properties from ENSDF, NUBASE-2012
- Update of average resonance properties for actinides (e.g. average spacing, strength function, $\Gamma\gamma$) if new evaluations available.

Planned CRP outputs

1) A technical document describing both the nuclear reaction formalism and model parameters included in the database.
2) A database will be made available for online distribution. All recommended parameters have to be tested using model calculations and compared with available reaction data, their inclusion into the database should be justified.

Planned CRP Goals

1) The following input parameters will be included into the database
   Fission parameters
   - Recommended set of empirical fission barriers (heights and widths) with estimated uncertainties
   - Recommended set(s) of theoretical barriers (including symmetries) and comparison with recommended empirical set to assess the predictive power
   - Recommended set(s) of class II/III states in the well(s) for accurate prediction of near threshold resonances for selected actinides (e.g. U-238, Th-232, Pa-231, etc.)
   - Recommended set(s) of transition states and tabulated level densities at the saddle points, and corresponding tabulated ground state level densities.

   Other input parameters
   - Recommended set(s) of optical model potentials for actinides
   - Optimized sets of gamma-ray strength functions for actinides including renormalization coefficients to describe available experimental data
   - Recommended set(s) of theoretical masses and ground state deformations
   - Updated set of discrete levels and decay properties from ENSDF, NUBASE-2012
   - Updated set of average resonance properties for actinides (e.g. average spacing, strength function, etc.) if new evaluations available.
2) Recommend sets of complete input parameter files for major codes optimized on the description (as coherent as possible) of available experimental cross sections for selected actinides (Coherence means to try to obtain unique set of fission input parameters for each fissioning nucleus independent of the fission chance and projectile). A typical input file may include fission barriers (including symmetries), class II/III states (and level densities) in the well(s) for accurate prediction of near threshold resonances, transition states and tabulated level densities at the saddle point, and corresponding ground state level densities.

Recommendations

1) To achieve the above-mentioned outputs we recommend starting a new IAEA CRP.
2) Calculated fission cross sections depend on input parameters, as well as on fission models and their implementation in existing reaction codes. To study the effects of different implementations using the same set of input parameters it is recommended to undertake a code inter-comparison of calculated fission cross sections before the CRP starts. The input data needed for code inter-comparison on fission cross-section calculations is detailed in Appendix 4.

3. SUMMARY OF THE PRESENTATIONS

Numerical simulations for low energy nuclear reactions including direct channels to validate statistical models, T. Kawano

Although significant efforts have been devoted to improve the reliability of the statistical Hauser-Feshbach model calculations, several open questions still remain for the neutron-induced reactions on actinides including fission. One of them is the width fluctuation model for a deformed system, where a strongly coupled channel exists. In the Hauser-Feshbach codes like EMPIRE, TALYS, CCONE, and CoH3, a simplified method is employed in which the direct reactions are subtracted from the neutron transmission coefficients and perform the statistical model calculations just like a spherical nucleus case.

Kawano presented a numerical simulation for the statistical nuclear reaction models for such cases. This model basically simulates neutron-induced reactions on actinides in the fast energy range, in which the inelastic neutron scattering to the rotational band members occur strongly. While an actual cross-section calculation is performed by the coupled-channels optical model and the statistical Hauser-Feshbach theory, our abstract model is constructed with the so-called stochastic scattering matrix based on the Gaussian Orthogonal Ensemble (GOE). Unlike the K-matrix simulation performed by Moldauer or Hofmann et al., random variables appear in the energy denominator only, and the randomness in the decay amplitudes is given by the orthogonal transformation of the stochastic scattering matrix into the K-matrix.

Including the off-diagonal components in the back-ground S-matrix as the direct channel, the ensemble average of the simulated cross sections are compared with the statistical models. Two models are considered; (1) the direct channel flux is subtracted from the transmission coefficients and standard Hauser-Feshbach calculations with the width fluctuation correction are performed (this emulates the usual Hauser-Feshbach codes), and (2) the energy-averaged S-matrix is first diagonalize to eliminate the off-diagonal elements (Engelbrecht-Wedenmueller transformation), and the Hauser-Feshbach with width fluctuation is performed in the channel-space. The numerical simulation for 100 resonances and 3 channels showed that there is no significant difference between (1) and (2). However, the simulation results are preliminary, and more simulations including different number of resonances and channels should be performed.

Towards predictions of fission cross sections, S. Goriely

Detailed fission paths have been recently determined on the basis of the HFB model which has proven its capacity to estimate the static fission barrier heights with a relatively high degree of accuracy [1]. The barriers determined within the HFB-14 model [1] reproduce the 52 "empirical" primary barriers (i.e. the highest barriers of prime interest in cross section calculations) of nuclei with $88 \leq Z \leq 96$ with an rms deviation as low as 0.67 MeV. A similar accuracy is obtained (0.65 MeV) for the secondary barriers. Similar or higher rms deviations on empirical barriers are found by the microscopic-macroscopic approaches [2,3]. However, when dealing with exotic neutron-rich nuclei large differences are found in the predictions, HFB-14 barriers being in general relatively higher.

Such HFB calculations also provide all the necessary ingredients to estimate the nuclear level densities (NLD) within the combinatorial approach [4]. On the basis of the single-particle scheme and pairing strength of the same HFB-14 model that was used to determine the HFB-14 mass table and the fission path, a very satisfactory prediction of NLD in the ground state configuration is obtained at the neutron binding energy for both the s- and p-wave data [4].

The very same model has been used to estimate coherently the spin- and parity-dependent NLD at the fission barriers on the basis of the HFB-14 single-particle level scheme and pairing strength at the corresponding deformations of both the inner and outer saddle points.
The above-mentioned fission ingredients have been tested in neutron-induced fission cross section calculations [5,6]. For data evaluation purposes, it is possible to adjust the nuclear ingredients to reproduce at best the cross sections. In particular, the inner and outer barrier heights can be scaled coherently, without modifying the fission path topology, and the NLD at each saddle points renormalized in a way similar as done with the ground state NLD [4]. It was possible to achieve a satisfactory adjustment on all observables for the U chain in the 1 keV to 30 MeV range making a coherent use of one unique set of renormalization parameters independently of the channel or target considered and with a number of free parameters about five times smaller than the number of renormalization parameters used in the evaluation based on phenomenological inputs. Microscopic models are, however, in essence very different than the phenomenological models traditionally used, so although similar fits to known data are achieved, non-negligible differences may be expected for nuclei, energy ranges, or reaction channels for which no data exist.

Turning to the *prediction* of fission cross section, if use is made of the default HFB fission paths and NLD, cross section can be estimated within more or less of factor of 10 with respect to experimental data [5]. The largest uncertainty obviously comes from the 0.5-1 MeV error bar on the barrier height and is inherent to all the existing barrier calculation. The factor of 10 can be reduced to a factor of 3 if the fission paths are globally renormalized by a constant factor depending on the even or odd number of nucleons [5].

Based on such a global renormalization procedure and the HFB fission input, all the spontaneous, β-delayed, neutron- and photo-induced reaction rates of astrophysical interest have been estimated for about 2000 nuclei with $90 \leq Z \leq 110$ lying between the valley of β-stability and the neutron drip line [7]. All fission rates have been coherently obtained on the basis of the same fission barrier penetration calculation predicted by the TALYS code.

Despite this first effort to determine coherently all the fission rates of astrophysical interest on the basis of a microscopic input model, improvements can be envisioned. These include:

- the improvement of the fission transmission coefficient calculation in TALYS to take the direct contribution below the barrier into account;
- the estimate of all the fission inputs (fission path and corresponding NLD at the saddle points) within the Gogny-HFB approach based on the D1M interaction in collaboration with Bruyères-le-Chatel;
- the coherent adjustment of the microscopic inputs (path, NLD) on more experimental data as already performed on the U chain;
- the calculation of the β-delayed fission with the HFB input for fission and HFB+QRPA β-decay strength and the comparison with new experimental data.

[1] Goriely, S., Samyn, M., and Pearson, J.M., 2007, Phys. Rev. **C75**, 064312.
[2] Moller, P. et al., 2009, Phys. Rev. **C79**, 064304
[3] Myers and W.D., Swiatecki, W.J., 1999 Phys. Rev. **C60**, 014606.
[4] Goriely, S., Hilaire, S., and Koning, A.J. 2008, Phys. Rev. **C78**, 064307.
[5] Goriely, S., Hilaire, S., Koning, A.J., Sin, M., and Capote, R. 2009, Phys. Rev. **C79**, 024612
[6] Goriely, S., Hilaire, S., Koning, A.J., and Capote, R. 2011c, Phys. Rev. **C83**, 034601.
[7] Xu, Y., Goriely, S., Jorissen, A., Chen, G.L., Arnould, M. 2013,
Astronomy & Astrophysics **549**, A106. See also http://www.astro.ulb.ac.be/bruslib.

Some requests for RIPL, Osamu Iwamoto

Comments from the members of Nuclear Data Center at JAEA were presented. Generally speaking, the present RIPL database is almost satisfactory. It is very useful for nuclear data evaluation. The CCONE code, which has been developed at JAEA, integrates the RIPL database and was successfully used for JENDL-4 evaluation. However, there are some requests for RIPL and listed flowing:

- release of the tool to create RIPL level database from ENSDF is desired to keep the data up-to-date by RIPL users,
- band information is desired in the level scheme to be used for coupled channel calculation,
- GDR parameters which are well fitted to experimental data depending on gamma-ray strength functions are desired,
- more comprehensive OMP database is desired including such as Kunieda's OMP.

TALYS-1.6, A. Koning

A presentation is given on the new features included in the new TALYS release. As usual after 2 years of development, TALYS-1.6 was released 23 December 2013. Figures 1 and 2 show the worldwide use of the code so far, represented in number of publications per year and per application area.

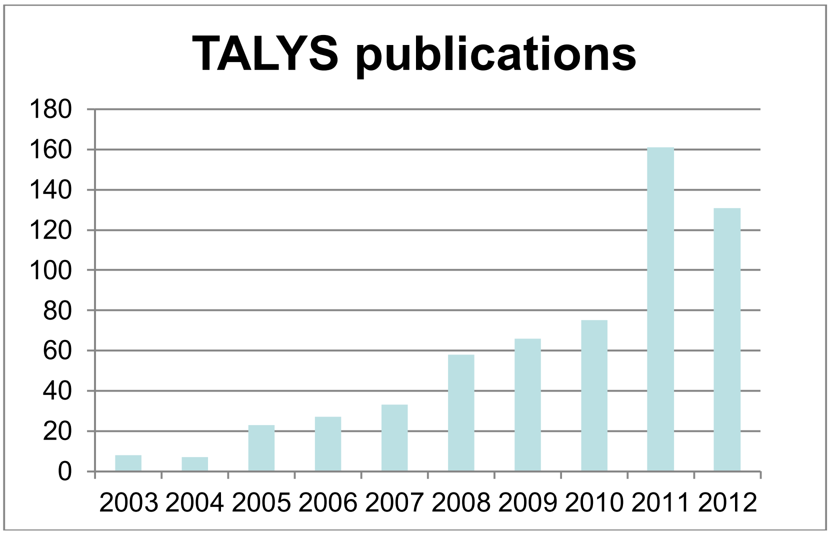
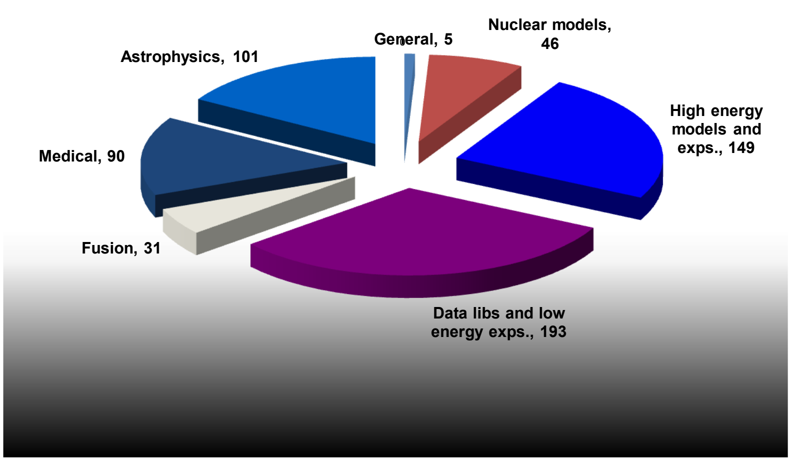
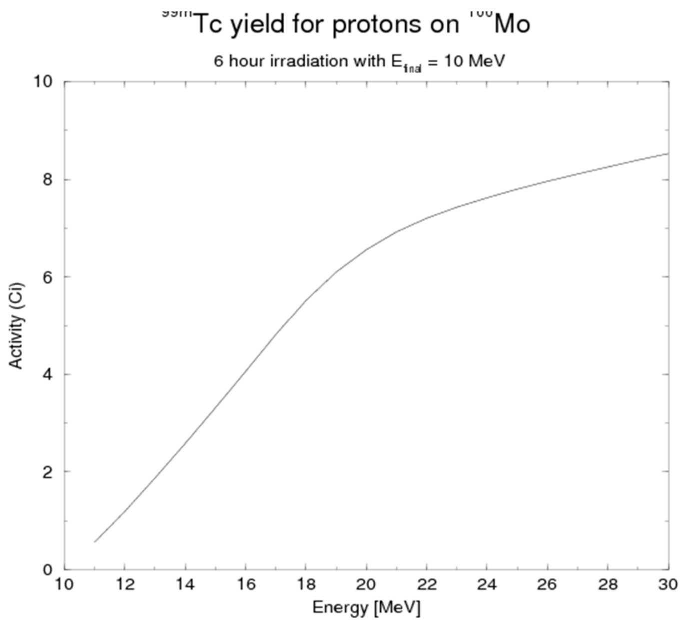


Figure 1: Number of publications (top) and worldwide use of TALYS (bottom)



Compared to the previous release, 1.4, the code contains 4 main new features:

- Direct neutron capture, see Xu and Goriely, "Systematic study of direct neutron capture", Phys. Rev. C86, 045801 (2012).
- Medical isotope production using accelerators: Integration of all excitation functions over incident energy to provide all radioactive production yields, in Ci or GBq (also per mAh), specific activities and impurities. All accelerator characteristics like energy, current, cooling time, etc. can now be provided to TALYS, see Figure 2.
- Fission yield and neutron multiplicities using the GEF model of Schmidt and Jurado, implementation by Simutkin and Onegin. TALYS-1.6 now provides FY(Z,A), P(nu), nubar(Z,A) and total nubar, see Figure 3.
- Extension to 1 GeV. The Koning-Delaroche OMP has been extended by simple phenomenological forms to provide good total and reaction cross sections up to 1 GeV. In addition, logarithmic excitation energy binning was included in the multiple Hauser-Feshbach decay, see Figure 4.



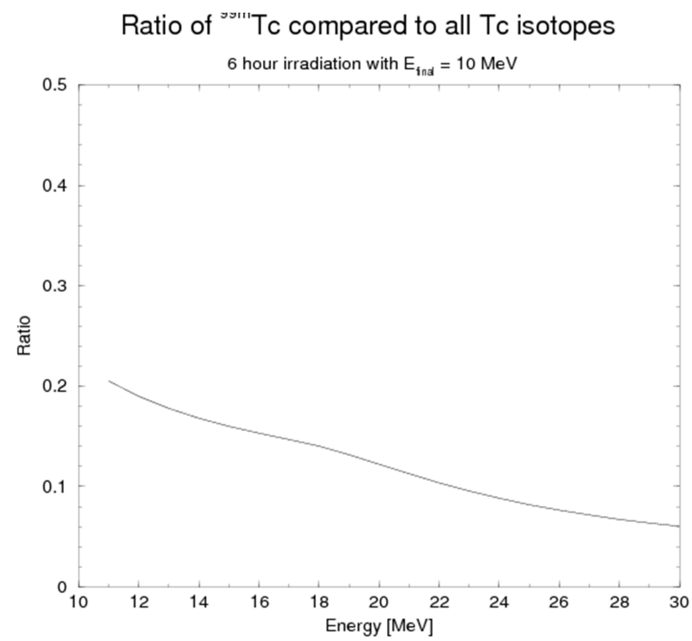
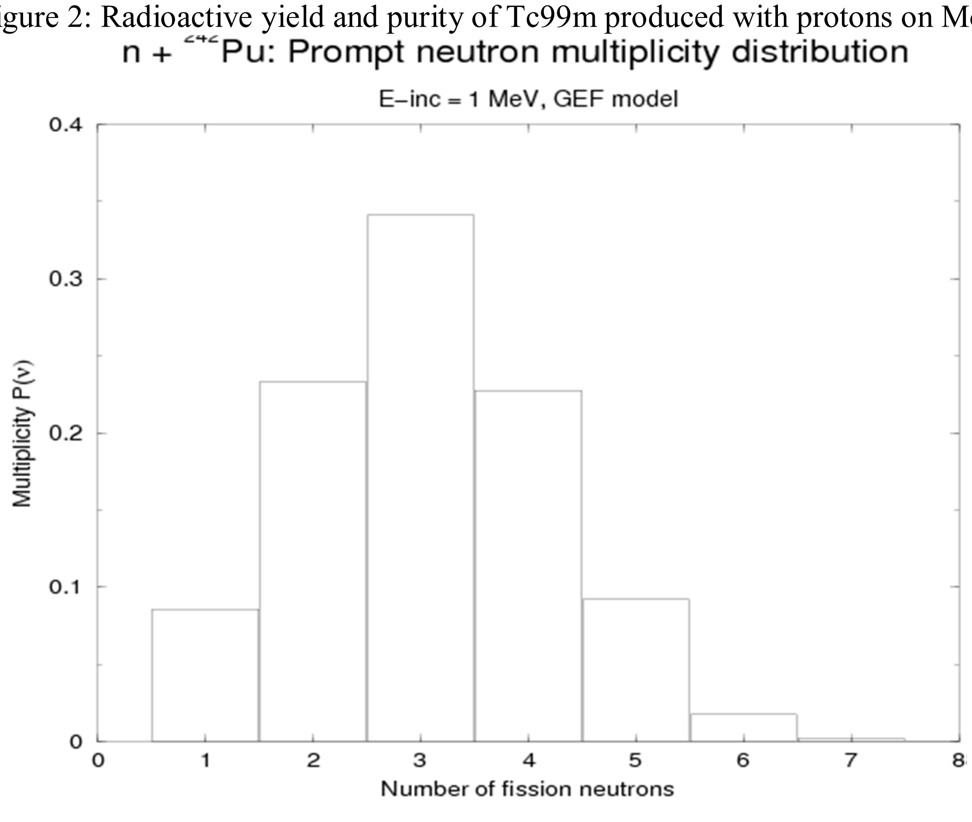


Figure 2: Radioactive yield and purity of Tc99m produced with protons on Mo100.



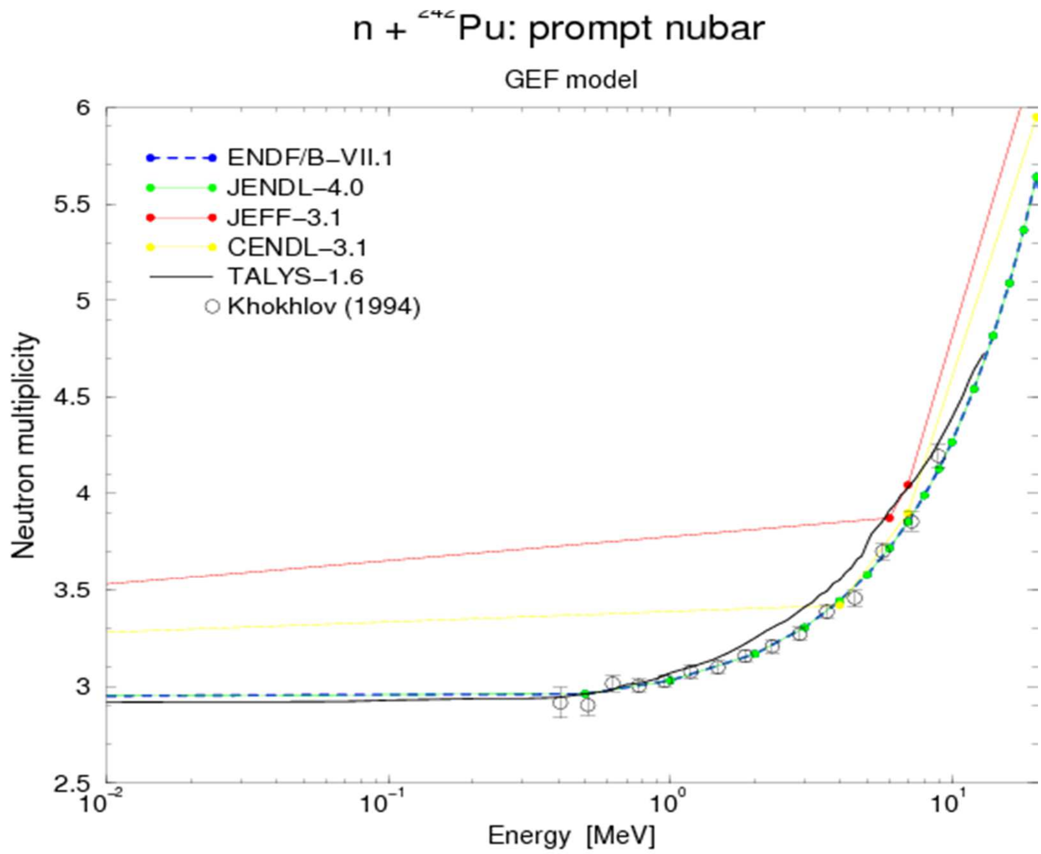
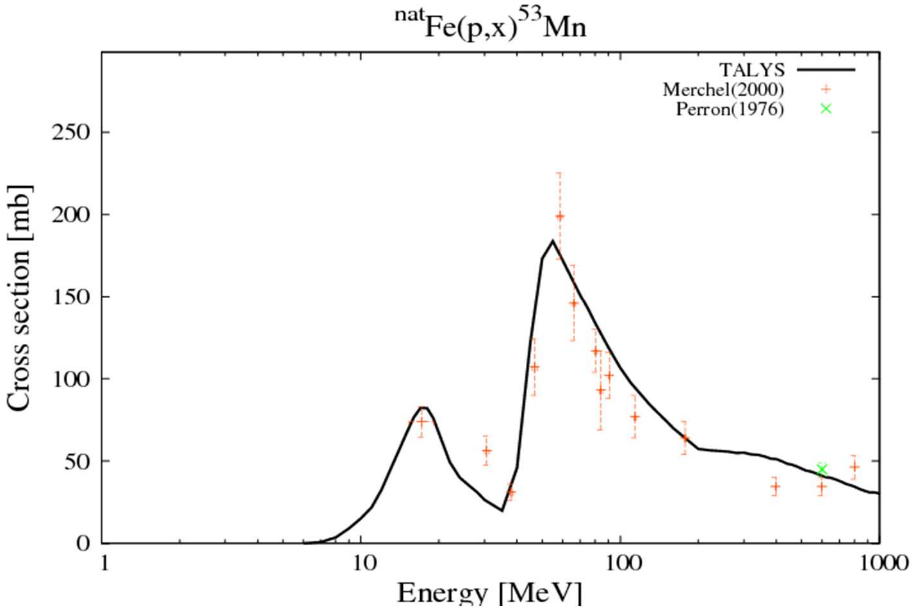


Figure 3: Prompt neutron multiplicity distribution and average neutron multiplicity for neutrons on Pu-242



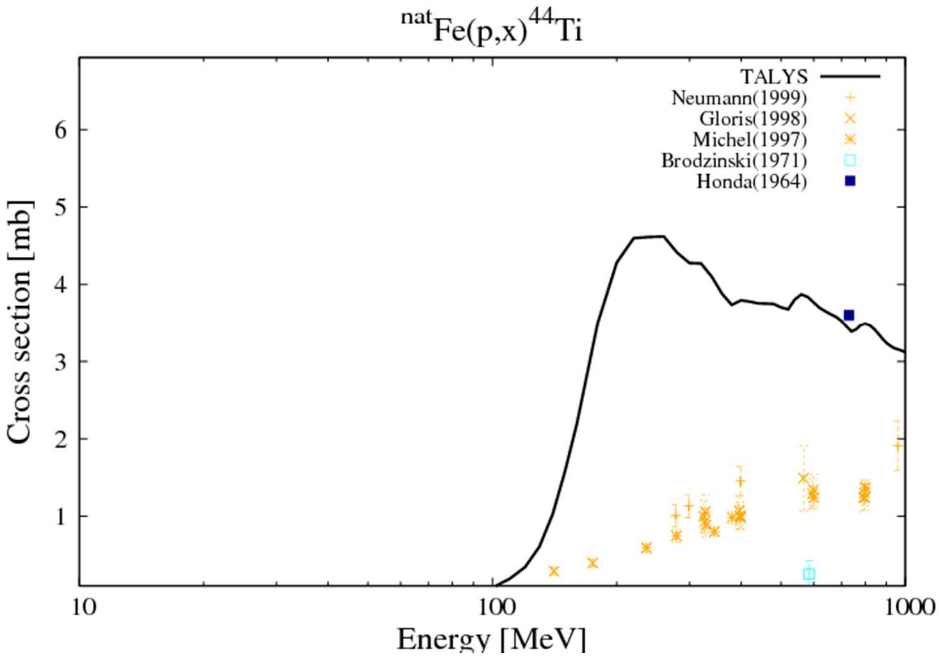


Figure 4: Reactions up to 1 GeV with TALYS-1.6.

The plans for TALYS-2.0 are outlined: This will include the codes TASMAN, for uncertainties, covariances and sensitivities, and TEFAL, for ENDF-6 formatting, fully integrated in a new Fortran95+ program.

TALYS and RIPL, A. Koning

Here is an outline of recent or upcoming issues of the various RIPL segments, related to TALYS:

- Masses. This is a rather stable segment, only updated HFB tables from either Brussels (Skyrme) or Bruyeres (Gogny) are added.
- Discrete levels: In 2013, a new RIPL discrete level database was adopted for TALYS, and a after a few rounds of feedback a frozen version was included in TALYS-1.6. In 2014, a new version prepared by IAEA, solving various issues of rotational bands and ground state assignment, will be tested and probably adopted for the next version of TALYS. The current RIPL database is used as TALYS reference for nuclides: TENDL-2013 contains 2626 targets, which are all nuclides in either ground or isomeric state with half-life longer than 1 sec. TALYS also has tables with spectroscopic factors per level for direct capture.
- Neutron resonance parameters: Nothing to report
- Optical model parameters: TALYS will include the RIPL OMP segment as an interface. The TALYS database also has complete coupled-channels coupling schemes for about 200 nuclides, enabling automatic ECIS calculations for deformed nuclides
- Level density parameters: No new developments on model and parameters. However, TALYS will have an extra output option to tabulate the level densities for the fission barriers, so that the foreseen exercise of comparing fission cross section calculations can be done.
- Gamma-ray strength functions: Nothing to report.
- Fission: TALYS has the same problem as other codes seem to have – it is difficult to perform consistent cross section calculations for actinides, based on just published parameters. Therefore, as mentioned above, level densities will be tabulated and used as input for fission calculations.

Update of the RIPL discrete level database, M. Verpelli

On-going efforts to update the Nuclear Levels Segment of the Reference Input Parameter Library (RIPL) were described. The updated library addresses the issue of levels with unknown energy, extends the Ground States properties with Nubase2012 data, and calculates the Internal Conversion Factor of gamma transition using BrIcc. The software implementation relies on a relational database. The updated library is undergoing validation in nuclear model calculations.

APPENDIX 1. AGENDA

Consultants' Meeting on

Recommended Input Parameters for Fission Cross Section Calculations

IAEA Headquarters, Vienna, Austria
17 – 18 December 2013

Meeting Room M0E13

AGENDA

Tuesday, 17 December

08:30 - 09:30	**Registration** (IAEA Registration desk, Gate 1)
09:30 - 10:00	**Opening Session**
	Introduction – Roberto Capote Noy Adoption of Agenda
10:00 - 12:15	**Presentations by participants**
12:15 – 12:30	Administrative matters
12:30 – 14:00	***Lunch***
14:00 – 18:00	**Presentations by participants (cont'd)**

Coffee break as needed

Wednesday, 18 December

09:00 - 16:00	**Discussions and recommendations, review of the summary report**

Coffee and lunch break(s) in between

16:00	**Closing of the meeting**

APPENDIX 2. LIST OF PARTICIPANTS

Consultants Meeting on

"Recommended Input Parameters for Fission Cross Section Calculations"

BELGIUM
Stephane Goriely
Université Libre de Bruxelles
CP226, boulevard du Triomphe,
BE 1050, Brussels
Tel: +32 650 28 43
E-mail: sgoriely@ulb.ac.be

FRANCE
Stephane Hilaire
CEA/DAM, Ile de France B.P. 12
91680 BRUYÈRES LE CHÂTEL
FRANCE
Tel : +33 1 6926 6028
Fax: +33 1 6926 7063
Email: stephane.hilaire@cea.fr

NETHERLANDS
Arjan KONING
NRG Nuclear Research and
Consultancy Group
Westerduinweg 3
PO Box 25
1755 ZG Petten
Tel: +31 224 564051
E-mail: koning@nrg.eu

JAPAN
Osamu Iwamoto
Nuclear Data Center
Japan Atomic Energy Agency
Tokai-mura, Naka-gun
IBARAKI-KEN 319-1195
Tel. +81 282 5483
E-mail: iwamoto.osamu@jaea.go.jp

USA
Toshihiko Kawano
T16, MS B243, Theoretical Division
Los Alamos National Laboratory
LOS ALAMOS, NM 87545
Tel: + 1 505 664 0513
E-mail: kawano@lanl.gov

IAEA
NAPC Nuclear Data Section
Vienna International Centre
PO Box 100
1400 Vienna, Austria
Fax +43-1-2600 7

Roberto CAPOTE NOY
Tel. +43-1-2600-21713
E-Mail: r.capotenoy@iaea.org

Stanislav SIMAKOV
Tel. +43-1-2600 21717
E-mail: s.simakov@iaea.org

Marco VERPELLI
Tel. +43-1-2600 21723
E-mail: m.verpelli@iaea.org

APPENDIX 3. PHOTO OF MEETING PARTICIPANTS

From left:
Standing: S. Simakov, S. Hilaire, S. Goriely, M. Verpelli, O. Iwamoto, T. Kawano
Sitting : A. Koning, R. Capote, P. Dimitriou

APPENDIX 4. INPUT PARAMETERS FOR CODE INTER-COMPARISON OF FISSION CROSS-SECTION CALCULATIONS

Neutrons incident on two targets:
1) Fertile: U-238 (.1 to 5 MeV); 2) Fissile: Pu-239 (.1 to 5 MeV)

Incident energy grid: .1 (.1 step) up to 1 MeV; from 1. (.2 step) up to 5 MeV

- Do 1 run with no discrete transitional states, 1 with discrete transitional states
- Do 1 run with Width Fluctuation Correction, 1 without

We expect to receive a table containing all calculated cross sections including total, reaction, elastic (shape and compound separately), capture, inelastic and fission. The full (comprehensive) output of the calculations produced by the employed code could be also submitted to be used as a reference for the submitted calculations.

Deliver results to the IAEA by email (r.capotenoy@iaea.org) before 31st May 2015 using e.g. TALYS, EMPIRE, CoH3, and CCONE.

Input parameters:
RIPL 2601 = Soukhovitskii 2004 (5 CC)
RIPL-3 HFB LDs for ground states and saddles

Lorentzian GDR parameters for gamma-ray strength calculation (no additional normalization)

	E1	W1	E2	W2	N discrete levels
92 238 U	10.90	2.47	13.98	3.95	10
92 239 U	10.83	2.45	13.99	3.97	5
94 239 Pu	10.72	2.41	14.06	3.93	12
94 240 Pu	10.70	2.40	14.04	3.91	10

Fission barriers (double humped barrier -inner triaxial GA, outer – mass assymetric MA)

Fiss.Nucleus		Vi	HWi		Vo	HWo
92 238 U	GA	6.30	1.00	MA	5.50	0.60
92 239 U	GA	6.45	0.70	MA	6.00	0.50
94 239 Pu	GA	6.20	0.70	MA	5.70	0.50
94 240 Pu	GA	6.05	0.90	MA	5.15	0.60

Number of discrete vibrational band-head states at barrier 1 = 3 (Pu-240)

Jdis	Pidis	Edis	homega	h2/2J(A) = 0.005 MeV (Ecut = 1.20 – start of the continuum)
0.0	1	0.000	0.950	
2.0	1	0.300	0.950	
0.0	-1	1.100	0.950	

Number of discrete vibrational band-head states at barrier 1 = 3 (U-239)

Kdis	Pidis	Edis	homega	h2/2J(A) = 0.005 MeV (Ecut = 0.20 – start of the continuum)
0.5	1	0.000	0.660	
1.5	-1	0.020	0.680	
2.5	1	0.170	0.690	

Nuclear Data Section	E-mail: nds.contact-point@iaea.org
International Atomic Energy Agency	Fax: (43-1) 26007
Vienna International Centre, P.O. Box 100	Telephone: (43-1) 2600 21725
A-1400 Vienna, Austria	Web: https://www-nds.iaea.org