

PAUL SCHERRER INSTITUT



HORIZON
2020



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SANDA WP4: Report



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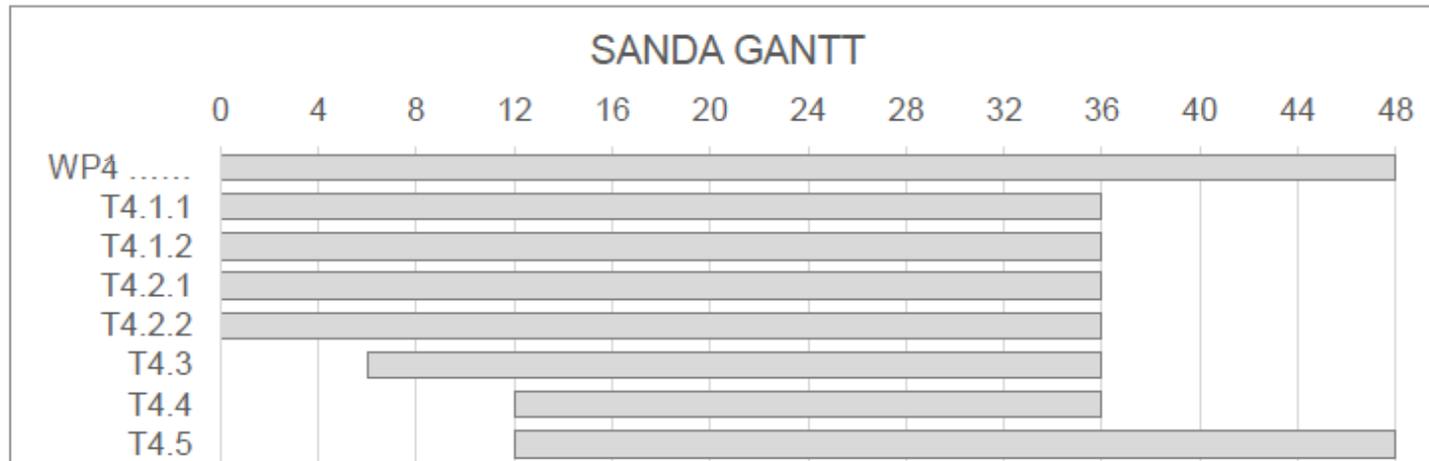
SANDA – review meeting, online, 30 November 2022



WP 4: Nuclear data evaluation

- WP description:

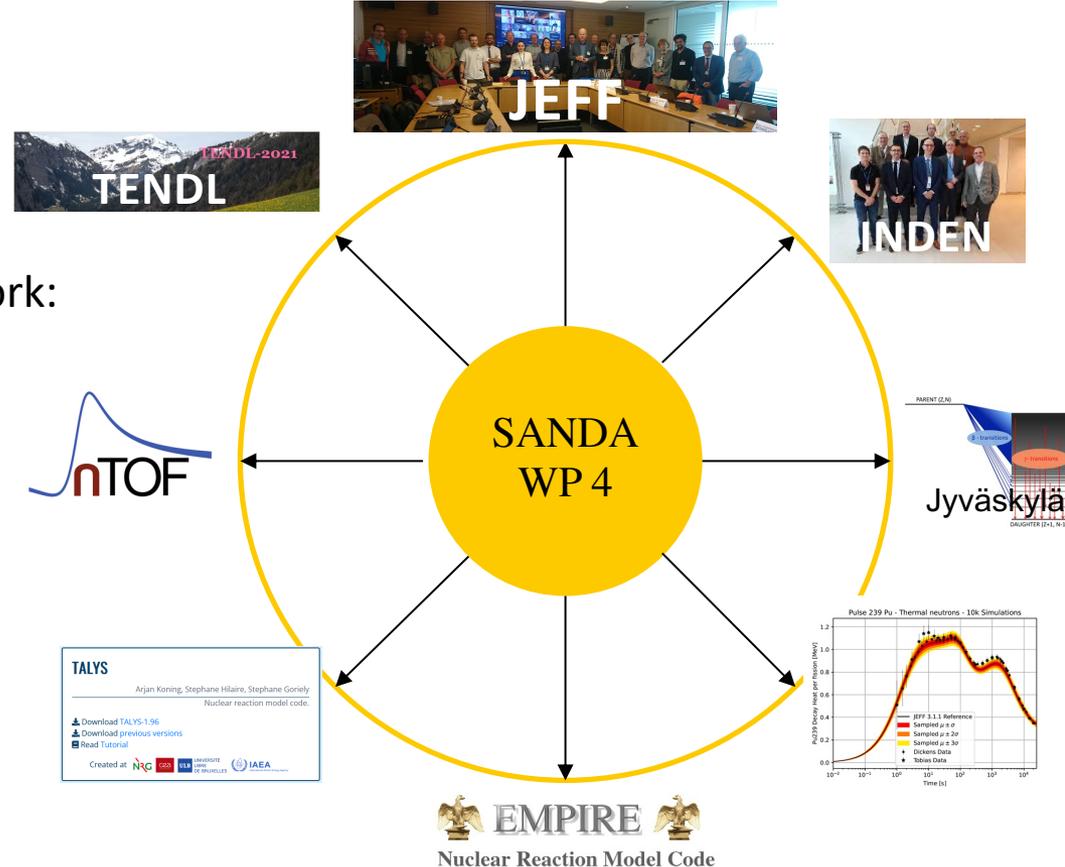
In this work package, it is proposed (1) to continue the development of open-source evaluation tools by improving the phenomenological and microscopic models (TALYS and EMPIRE for reaction nuclear data; and specific codes for decay and structure data, as well as fission yields), (2) to perform evaluation work for important isotopes (actinides and fission products, to be proposed to different international libraries), (3) to provide processed data ready to be used by simulation codes for validation purposes, (4) to provide sensitivity vectors for feedback analysis, and (5) to recommend a set of preferred systems (or benchmarks) for the validation of the new evaluations (see WP5).



- T0: September 2019
- T36: August 2022
- T48: August 2023

WP 4: Nuclear data evaluation

- This WP is crucial for:
 - European libraries:
 - OECD/NEA JEFF
 - TENDL
 - International libraries and network:
 - US CSWEG
 - INDEN
 - Key links to experimentalists
 - n_TOF
 - JRC Geel
 - Jyväskylä



- Allows communications, time and data exchange between evaluators (inside JEFF, NEA, IAEA)
- Delivering tools such as reaction codes (TALYS, EMPIRE)
 - Highly used in many fields: energy, astrophysics, medical, accelerators
 - Bring the latest theoretical developments to users

WP 4: Nuclear data evaluation

Work package 4				Lead beneficiary	PSI		
Work package title	Nuclear data evaluation and uncertainties						
Participant number	1	2	3	5	10	14	21
Short name of participant	CIEMAT	Atomki	CEA	CNRS	IFIN-HH	JSI	<i>PSI</i>
Person-months per participant	16.6	8.6	43.2	11.5	5	7.2	6
Participant number	24	25	26	32	33	35	
Short name of participant	Sofia	TUW	UB	UPM	USC	UU	
Person-months per participant	5.3	5	35	11.8	5	13	
Start month	1			End month	48		

- Main responsible persons:

- | | | | |
|------------|-----------------------|--------|--------------|
| – CIEMAT: | V. Bécares | – UB: | M. Sin |
| – Atomki: | J. Timár | – UPM: | O. Cabellos |
| – CEA: | G. Noguere et al. | – USC: | J. Benlliure |
| – CNRS: | M. Kerveno, M. Fallot | – UU: | H. Sjöstrand |
| – IFIN-HH: | A. Negret | | |
| – JSI: | I. Kodeli | | |
| – PSI: | D. Rochman | | |
| – Sofia: | S. Lalkovski | | |
| – TUW: | H. Leeb | | |

WP 4: Nuclear data evaluation

Table 3.1c: List of Deliverables⁴

4.1	Report on code development, methods	4	PSI	R	PU	40
4.2	Report on new nuclear reaction data evaluation	4	CEA	R	PU	48
4.3	Report on the evaluation for fission yields	4	CEA	R	PU	36
4.4	Report on the evaluation for nuclear structure and decay data	4	IFIN-HH	R	PU	36
4.5	Report on the processing and sensitivity analysis	4	UPM	R	PU	36
4.6	Report on the applications: recommendation	4	CIEMAT	R	PU	36
4.7	Report on the possibility to generalize the high-energy model uncertainties methodology	4	CEA	R	PU	48

T0: September 2019

T32: May 2022

T36: August 2022

T40: December 2022

T48: August 2023

Table 3.2a: List of milestones

Milestones:

M.4.1: availability of TALYS modules (CEA/DAM/DIF): M32

M.4.2: availability of new EMPIRE modules/models (UB): M32

M.4.3: availability of evaluated files for important actinide isotopes (CEA/DEN, CNRS): M32

M.4.4: availability of evaluated files for important fission products (CEA/DEN, PSI): M36

4.1	Availability of TALYS modules	4	32	Short communication
4.2	Availability of new EMPIRE modules/models	4	32	Short communication
4.3	Availability of evaluated files for important actinide isotopes	4	32	Presentation or ENDF file
4.4	Availability of evaluated files for important fission products	4	36	Presentation or ENDF file

Task 4.1: Nuclear reaction code developments and evaluations

Task coordinator: PSI, partners: CEA/DAM/DIF, CEA/DEN, PSI, CNRS/IPHC, TUW, UB, UU

Task 4.1.1: TALYS development

The development of TALYS for better modelling and its associated model parameter database will be performed within the TALYS collaboration (IAEA, PSI, ULB). Examples of important observables are the spectra and multiplicities of gamma and neutron. They are essential for nuclear applications such as criticality but also for shielding. In this context, efforts on statistical decay of fission fragments using TALYS were initiated during the ANDES project, and continued during the CHANDA project. For this new

Task 4.1.2: Nuclear reaction evaluation

Prior the production of nuclear reaction evaluations (in the form of ENDF files), different methods will be studied and compared. CEA/DAM, PSI and CEA/DEN will work together to improve evaluation methodologies for nuclear data and the associated uncertainties, by making use of Bayesian inference method with differential as well as carefully selected integral constraints. These groups have a large experience in ENDF file productions.

These applied methods can be complemented by “model defect” methods, as presented by TUW. TUW is

See examples in the next slide

Subtask 4.1: examples

1. TALYS publicly released in December 2021 (on two independent websites)
2. Latest theoretical TALYS implementation being currently tested (on schedule)
3. EMPIRE publicly released in November 2021
4. Unique development for light isotopes (GECCOS code)
5. Presented in the JEFF general meetings, at the ND2022 international conference and at the CW2022 international workshop.
6. TENDL-2021 (and 2023), JEFF-4.0 heavily supported by SANDA evaluations (U235, U238, Pu239, Xe135, Cs133, Ag107, Ag109, Eu151, Eu153, Eu154, Eu155, Lu173, Lu175, Lu176, Pm148m and Pu238)
7. Common work between
PSI, IAEA, CEA, UB, UW

TALYS

TALYS-Related Software and Databases

TALYS and the TALYS-related packages are open source software and datasets ([GPL License](#)) for the simulation of nuclear reactions.

TALYS

Arjan Koning, Stephane Hilaire, Stephane Goriely
Nuclear reaction model code.

[Download TALYS-1.96](#)
[Download previous versions](#)
[Read Tutorial](#)

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Task 4.2: Fission yields and nuclear structure and decay data evaluations

Task coordinator: IFIN-HH, partners: IFIN-HH, CEA/LNHB, CNRS/LPSC, Sofia, Atomki, CNRS/Subatech

Task 4.2.1: Evaluation of Fission yields

The analysis and evaluation of fission yields is also of prime importance for many applications (*e.g.* correct estimation of the content of spent nuclear fuel). The CEA/DEN, CNRS/LPSC and ILL have a large experience in measuring, analysing and evaluating thermal neutron-induced fission yields. In the framework of a collaboration between the Physical Studies Laboratory (LSP) of the CEA Cadarache (France), the

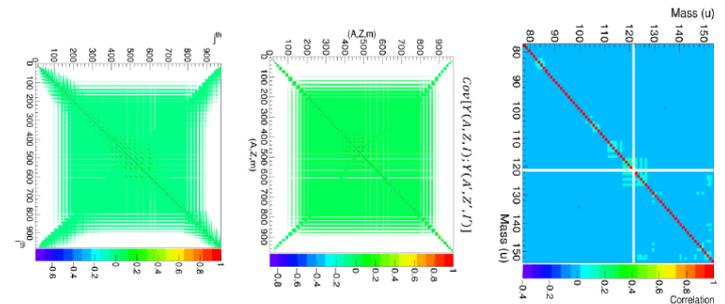
Task 4.2.2: Evaluation of nuclear structure and decay data

Together with the fission yields, evaluations of nuclear structure and decay data can have an important impact on specific applications, such as decay heat calculations. Additionally, it is important that the (cumulative) fission yields are evaluated together with decay data. In this context, a few experienced groups will join efforts to perform ENSDF (Evaluated Nuclear Structure Data File) evaluations. ENSDF constitutes

See examples in the next slide

Subtask 4.2: examples

1. New fission yields for U-235 proposed to the JEFF community for the JEFF-4.0 library, available on gitlab
2. Considerable quality improvements, and answer user's need for covariances
3. Work presented at the JEFF meetings, ND2022, and CW2022
4. File testing based on SANDA collaboration
5. Work planned for Pu-239
6. New evaluations for decay data, first time financed in Europe.
7. Based on new experimental TAGS (Total Absorption Gamma Spectrometer) data at Jyväskylä
8. Measurements being analyzed by a PhD student (starting in Sept. 1, 2022).

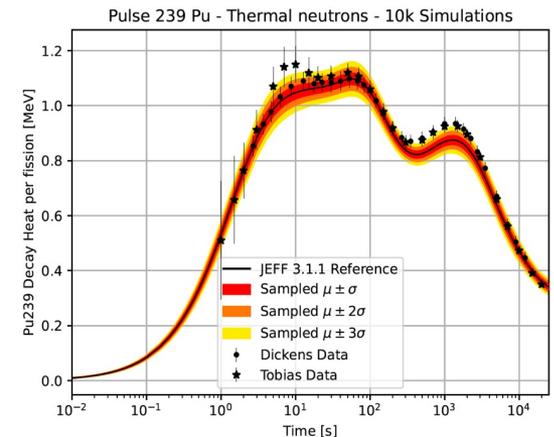
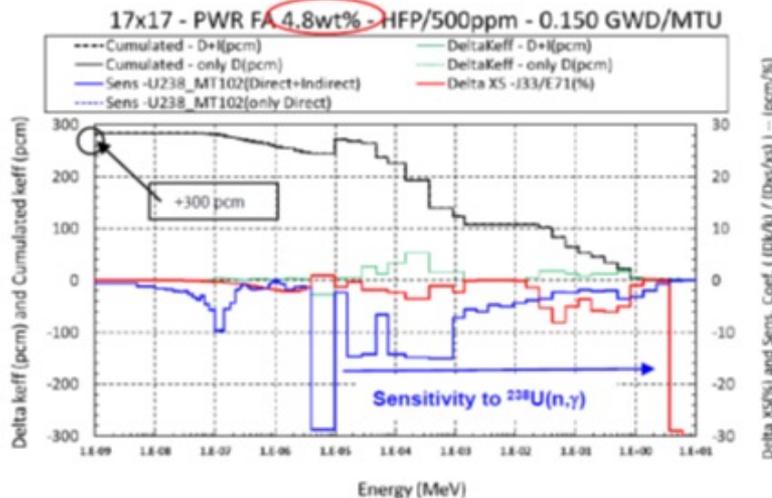


Task 4.3: Processing and sensitivity

Task coordinator: UPM, partners: CIEMAT, UPM, CNRS/Subatech

The processing step is strongly linked to the evaluation process and allows basic evaluations (in the ENDF-6 format) to be used by a variety of simulation codes. In the CHANDA project (Task 9.4), quality-assured processing routes for PREPRO and NJOY nuclear data processing codes were established; however, the AMPX code system was neglected because AMPX was not freely distributed with SCALE at that time. As a

1. Verification and correction of the AMPX processing (now available at the NEA), test with JEFF-4.0T0
2. Testing and processing with NJOY2016 (presented at JEFF sessions and WPEC/SG46)
3. Sensitivity for burnup & shielding calculations
4. Impact of fission yields uncertainties on decay heat calculations



Task 4.4: Applications

Task coordinator: CIEMAT, partners: UPM, CIEMAT, JSI

To complete this work package and provide a suitable link with the Work Package on validation (WP5), recommendations for preferred benchmark for thermal and high energy (up to 20 MeV) will be proposed. Whereas nuclear data validation has been in the recent years mostly restricted to critical benchmarks, this effort will also focus on other types of measurements, such as shielding benchmarks and kinetics. The code such as SUS3D (ISD) will be used for shielding calculations with improved S/U analysis of the impact of the

1. Benchmarks for kinetic parameters
2. Improvements of the SINBAD shielding benchmarks (available at the NEA), helping for Fe, Cu validations for the new nuclear data libraries
3. Improvements of the SINBAD depletion benchmarks and spent fuel benchmarks (e.g. SFCOMPO, available at the NEA)

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	REF. EXTERNA	REVISION 0

TITULO: Review of available benchmark experiments for kinetic parameter validation

AUTORES: V. Bécáres, J. Llanes-Gamonoso, S. Panizo, A. Sánchez-Caballero, D. Álvarez-Fernández

ABSTRACT:

This report presents the results of the work performed by CIEMAT within SANDA Task 4.4. We have performed a bibliographic search (ICSBEP and IRPhE databases and the scientific literature) for nuclear reactor benchmark experiments containing experimental information about kinetics parameters, namely the effective delayed neutron fraction (β_{eff}), the effective mean neutron generation time (Λ_{eff}) and the prompt neutron decay constant (α). This report presents the results of this search. Furthermore, to determine the level of sensitivity to nuclear data of these parameters, S/U analyses have been performed with the SUMMON code alongside with sensitivity coefficients calculated with the MCNP 6.2 code (KSEN card) and the JEFF-3.3 nuclear data library. For uncertainty quantification, covariance matrices from ENDF/B-VIII.0, JEFF-3.3 and JENDL-4.0u have been used.

Task 4.5: High-energy model uncertainties

Task coordinator: CEA/Saclay, partners: CEA/Saclay, USC

Finally, the higher energy part (above 20 MeV) and especially the propagation of uncertainties from the high-energy models (and parameters) will be studied (CEA/Saclay, USC). Codes used for the simulation of Accelerator-Driven Systems (ADS) and for number of other applications, such as for instance radiation

1. Calculations of high relevance for accelerator developments, as well as high energy beam simulation in space.
2. Current developments are for uncertainty calculations, following the developments in the CHANDA project
3. Combination of Bayesian calculations coupled with Taylor expansion
4. Work under development and according to schedule

Status of milestones

- MS30: Availability of TALYS modules
 - Due on 30/04/22,
 - Done on 15/12/21
- MS31: Availability of new EMPIRE modules/models
 - Due on 30/04/22,
 - Done on 30/11/22
- MS32: Availability of evaluated files for important actinides
 - Due on 30/04/22,
 - Done on 30/11/22
- MS33: Availability of evaluated files for important fission products
 - Due on 30/04/22,
 - Done on 30/09/22

Status of deliverables

- D4.1: Report on code development and methods
 - Due on 31/12/22,
 - Expected to be done with delays before the next JEFF meeting (06/2023)
- D4.2: Report on new nuclear reaction data evaluation
 - Due on 31/08/23,
 - Expected on time
- D4.3: Report on evaluation for fission yields
 - Due on 31/08/22,
 - Expected 31/08/23
- D4.4: Report on the evaluation for nuclear structure and decay data
 - Due on 31/08/22,
 - Expected 31/08/23
- D4.5: Report on the processing and sensitivity analysis
 - Due on 31/08/22,
 - Expected 31/08/23
- D4.6: Report on the applications: recommendation
 - Due on 31/08/22,
 - Expected 14/10/22 (draft report submitted)
- D4.7: Report on the possibility to generalize the high-energy model uncertainties methodology
 - Due on 31/08/23
 - Expected on time

Explanation for delays

- D4.1: Report on code development and methods (6 months delay)
 - Delays from the experimental facility and start of PhD (COVID)
- D4.2: Report on new nuclear reaction data evaluation (no delays foreseen)
- D4.3: Report on evaluation for fission yields (1 year delay)
 - Unexpected feedback from evaluation developments, discussion with experts and adjustment on methods. But task partly performed and very positive developments
- D4.4: Report on the evaluation for nuclear structure and decay data (1 year delay)
 - Due to experimental activities (start of PhD on 01/09/2022): Subatech, and Jyväskylä.
- D4.5: Report on the processing and sensitivity analysis (1 year delay)
 - Delays due to adjustment on other projects (NEA Git, benchmark, JEFF4-T releases)
- D4.6: Report on the applications: recommendation (2 months delay)
 - Draft report delivered, under reviewed.
- D4.7: Report on the possibility to generalize the high-energy model uncertainties methodology
 - (no delays foreseen)

Conclusions

- WP allows to articulate collaboration between many European institutes
- A large number of outcomes (codes, presentations, papers, evaluated files)
- Important collaboration with international institutions (NEA, IAEA) and strong links institutes outside the EU (US, Japan)
- Outcomes used in energy application, astrophysics, accelerator technology
- Support both applied and theoretical developments
- Some delays due to COVID (PhD student not available & experimental facility not available)

Wir schaffen Wissen – heute für morgen

