Nuclear Data Activities of the EUROfusion Consortium

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Outline

- Background
- DEMO and IFMIF-DONES
- Neutronics simulations in fusion technology
- Nuclear data for fusion applications
- Nuclear data in EUROfusion/PPPT
- Summary & Outlook

Background

- **European Fusion Roadmap**
  - Realization of fusion as energy source for electricity by ~2050

    ⇒ *Fusion Power Plant (FPP) providing electricity to the grid*
  - Eight missions, three major facilities: ITER, DEMO, neutron source
  - **EUROfusion** Consortium for the Development of Fusion Energy in Europe

    ⇒ ***Power Plant Physics and Technology (PPPT)*** *programme*
- **DEMO power plant**
  - Conceived as single step between ITER and commercial FPP
  - Demonstrate ***tritium*** *breeding capability, production of* ***net electricity****, all* ***technologies*** *required for the construction of commercial FPP*
- **D-Li neutron source IFMIF-DONES**
  - Provide material irradiation data required for the construction of DEMO

⇒ ***Implemented in PPPT projects including design activities & supporting R&D***

PPPT projects

- **PMI –System Engineering, Design and Physics Integration**
- **BB – Breeder Blanket**
- **SAE – Safety and Environment**
- **MAT – Materials**
- DC – Diagnostic and Control
- DIV – Divertor
- RM – Remote Handling
- **ENS – Early Neutron Source**
- S2 – Stellarator Engineering

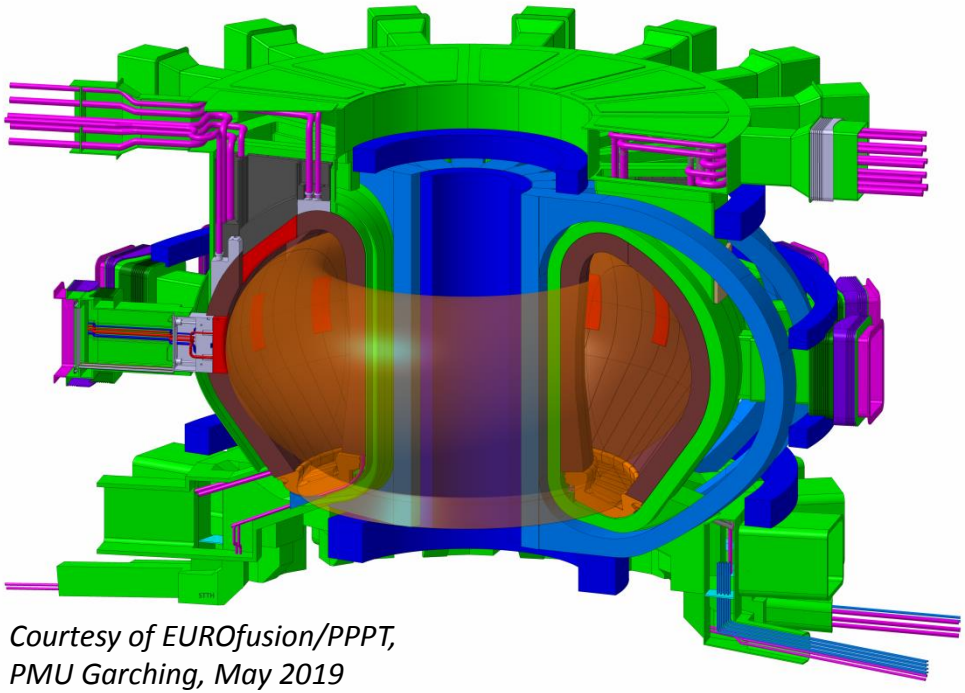
Neutronics serves all these projects:

⇒ ***Provides data required for nuclear design of plant, systems & components***

⇒ ***Evaluate & proof nuclear performance incl. licensing & safety related issues***

DEMO 2017 Baseline

"EU DEMO1 2017"
Cut-away CAD model



Courtesy of EUROfusion/PPPT, PMU Garching, May 2019

Main reactor parameters	
No. of TF coils	16
Major radius [m]	8.938
Minor radius [m]	2.883
Aspect ratio	3.1
Plasma elongation, κ_{95}	1.65
Plasma triangularitry, δ_{95}	0.33
Average neutron wall loading [MW/m^2]	1.05
Fusion power [MW]	1998
Net electric power [MW]	500

Neutronics - Issues & nuclear responses

- **Tritium breeding capability**
  - Tritium Breeding Ratio (TBR); net TBR ≥ 1.0
    ⇒ *To be evaluated, optimized and proven*
- **Nuclear power generation**
  - Total power produced in nuclear reactions, spatial distributions
    ⇒ *Reponses to be provided*
- **Shielding performance**
  - Radiation loads to superconducting magnets, structural and sensitive components/elements
    ⇒ *To be evaluated, optimized and proven*
- **Irradiation effects: Activation, transmutation, decay radiation**
  - Activity & nuclide inventories, decay heat, radiation damage to materials/components, radiation doses to materials & personnel
    ⇒ *To be evaluated & minimized – for operation, maintenance, safety, decommissioning and waste management*

⇒ ***Suitable computational approaches, tools and data needed to provide the required response data with sufficient accuracy.***

IFMIF-DONES Neutron Source

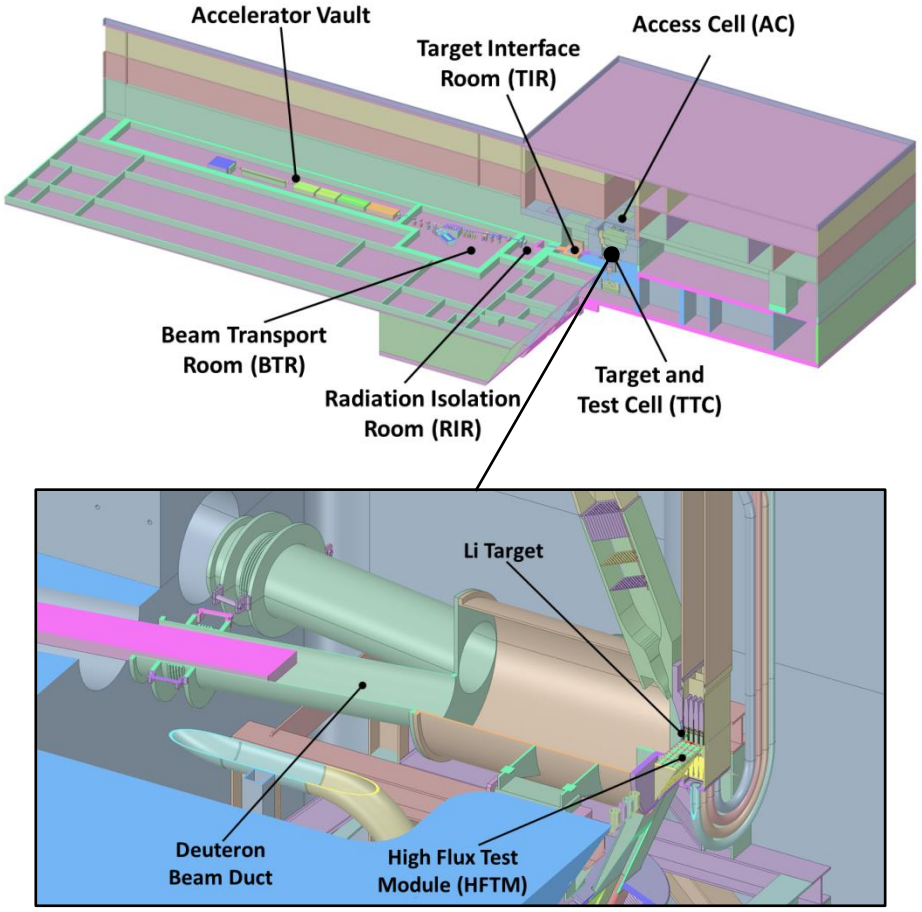
International **F**usion **M**aterial **I**rradiation **F**acility
Demo **O**riented **Ne**utron **S**ource

- **Early Neutron Source (ENS)** project of **EUROfusion** for a D-Li neutron source for material irradiations

⇒ ***Main mission**: To provide irradiation data for the construction of DEMO*

- Design based on IFMIF using only one deuteron accelerator (125 mA, 40 MeV)
- Lithium target, Test Cell and HFTM, etc. are (almost) identical, no other modules

⇒ ***Neutronics key issue:** Essential data to be provided for design, optimization, performance and safety evaluation*



IFMIF-DONES Neutron Source

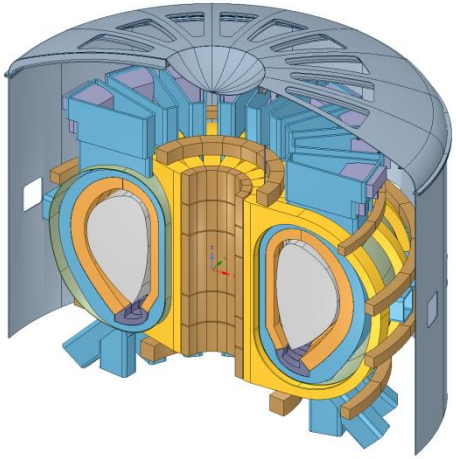
Major neutronics issues/tasks

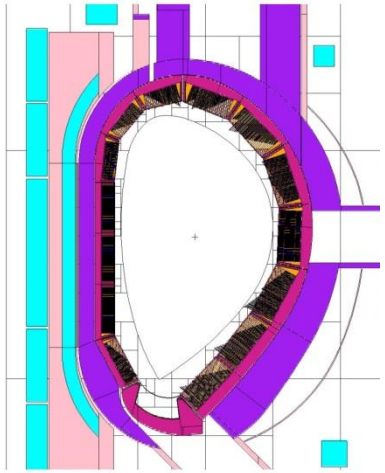
- D-Li neutron source producing neutrons up to 55 MeV – McDeLicious approach
- Nuclear performance of High Flux Test Module (HFTM)
  - *Neutron/photon flux distribution & spectra*
  - *Nuclear heating in HFTM container & specimens (Eurofer steel)*
  - *Radiation damage & gas production in specimens*
- Target & Test Cell (TTC)
  - *Nuclear design of Li target assembly, Li loop with quench tank, Test Cell with steel liner, concrete walls & plugs*
  - *Issues: nuclear heating (cooling), activation, radiation doses in/around TTC & Li loop during operation & maintenance ⇒ radiation maps*
- Accelerator System (AS)
  - *Radiation during operation due to deuteron beam losses and subsequent activation of AF components ⇒ deuteron transport (MCUNED code) & interaction with AF materials (activation, neutron generation)*
  - *Back streaming neutron radiation, shield design & optimization, beam dump*

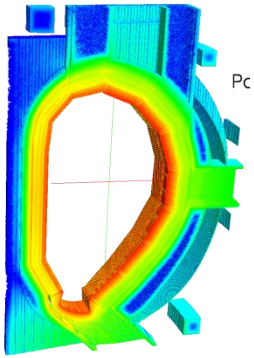
Neutronics simulations approach

Facility design → **Neutronics simulation** → **Nuclear responses**

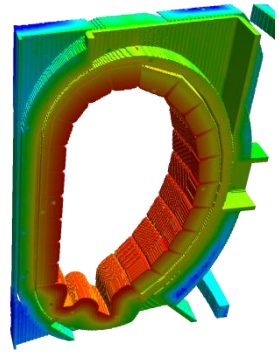
DEMO







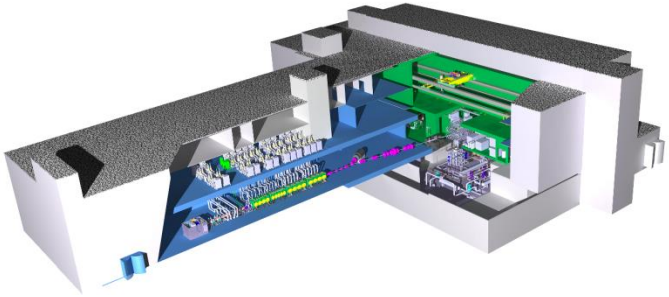
Nuclear heating

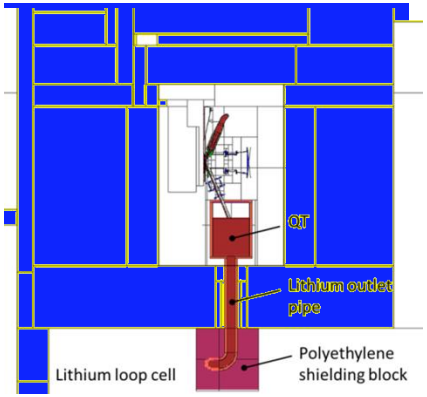


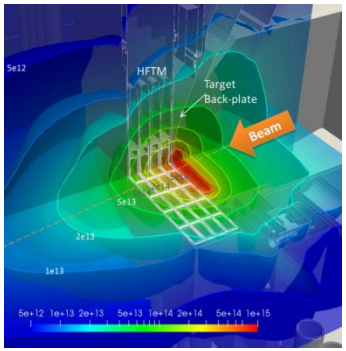
Decay gamma source

Tritium breeding, nuclear heating, activation & transmutation, radiation doses, …

IFMIF-DONES neutron source







Neutron flux

Nuclear heating

Displacement damage, gas production, nuclear heating, radiation doses, …

Neutronics simulations approach

- **Neutron (and photon) transport simulations**
  - Basis for providing all **nuclear responses** needed for the design and performance evaluation of fusion technology facilities.
  - Suitable computational approaches, tools and data required:
    - Method/tool for simulation of neutron transport in complex 3D geometry

    ⇒ *Monte Carlo (MC) particle transport technique (MCNP, TRIPOLI, Serpent, etc.)*
    - **Nuclear cross-section data** to describe the nuclear interaction processes

- **Coupled activation and radiation transport calculations**
  - Basis for assessment of activity inventories and radiation fields after shut-down as required for safety, licensing, waste management
  - Computational approaches/tools and required:
    - Nuclide inventory calculation with coupling to particle transport
    - Large amount of neutron induced **activation cross-section data**

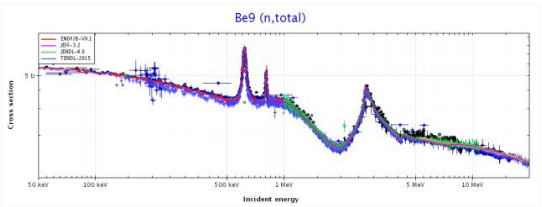
⇒ ***Neutronics simulations rely on variety and multitude of nuclear cross-section data and their quality !***

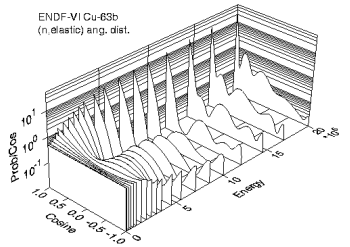
Nuclear data for fusion technology

- **Neutron cross-sections for transport simulations**
  - Neutron absorption and total cross-sections: $\sigma_a(E)$, $\sigma_{tot}(E)$
  - Total neutron emission cross-section $\sigma_{nem}(E,E',\mu)$

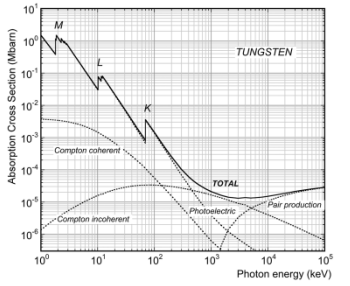
    [E = neutron energy, μ=cos(θ), θ=scattering angle]

    $\Rightarrow$ *Includes elastic scattering and inelastic reactions (n,n'γ), (n,2n),..*

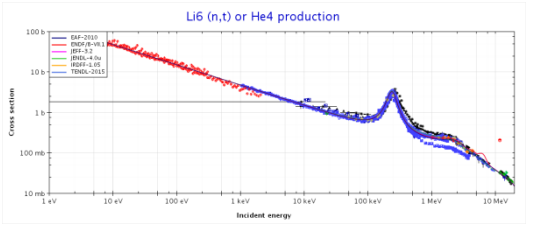




- **Cross-sections for photon transport simulations**
  - Neutron induced γ - production cross-sections and spectra
  - γ - interaction cross-sections



- **Nuclear data for calculating reaction rates ("nuclear responses")**
  - Cross-sections $\sigma_x(E)$ for specific reactions (tritium, gas production, etc.), and energy deposition (heating)



$\Rightarrow$ *<u>Complete data evaluations required</u> : all reactions, all data types, covering the entire energy range 10^{-3}eV – 20 MeV, for all nuclides of interest to FT, sufficient quality (!)*

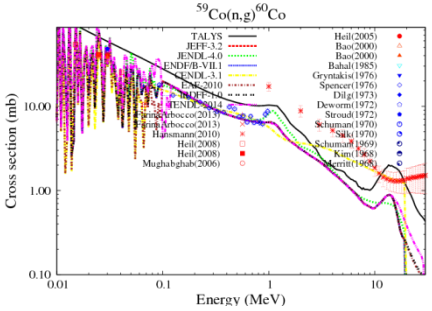
Nuclear data for fusion technology

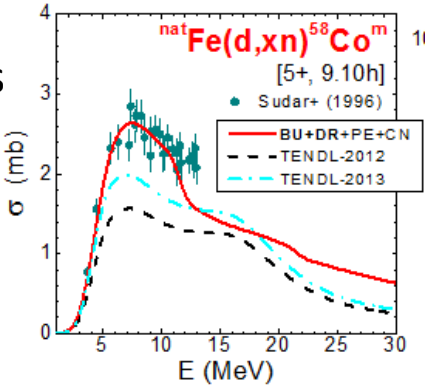
- **Nuclear data evaluations & libraries**
  - Evaluated nuclear cross-section data compiled in libraries, processed for application calculations, benchmarked and validated – as far as possible.
- **Nuclear data libraries for fusion technology**
  - **FENDL - Fusion Evaluated Nuclear Data Library**
    - Developed under auspices of IAEA, tailored to the needs of ITER
    - Current version FENDL-3.1d includes a set of sub-libraries, (n, p, d, activation, co-variances, etc.), up to 200 MeV
  - **JEFF - Joint Evaluated Fusion and Fission File**
    - Organised and maintained by NEA Data Bank, Paris, addressing needs of European nuclear fusion and fission communities
    - EU fusion data evaluations are fed into JEFF and its sub-libraries

⇒ ***JEFF serves as reference data library for PPPT nuclear analyses***

Nuclear data for fusion technology

- **Activation cross-section data**
  - Excitation function σ_x (E) for any open reaction channel producing a radioactive product nuclide
  - Calculated by nuclear model codes using experimental data, benchmarked and validated for important reactions
  - **European Activation File (EAF)** developed by CCFE/NRG in the frame of EU fusion programme, **serving both JEFF and FENDL**
  - **EAF- 2010** latest version (frozen): 816 target nuclides ^{1}H to ^{257}Fm, 66,256 excitation functions up to 60 MeV.
- **Deuteron induced cross-section data**
  - Required for IFMIF-DONES nuclear analyses
    - Neutron generation in Li target and accelerator components
    - Activation of deuteron beam facing materials of accelerator
  - TENDL deuteron library, based on automated model calculations





⇒ *To be updated with specific data evaluations/improvements*

Nuclear Data in EUROfusion/PPPT

- **Nuclear Data tasks implemented in PPPT programme**
  (starting 2017, previously conducted in Task Agreements with F4E, Barcelona, Spain)
  - ⇒ **To satisfy the needs for DEMO and IFMIF-DONES**
  - Transversal actions in PPPT projects PMI, BB, SAE, ENS, MAT
  - Starting in 2019, combined PMI task on "Nuclear Data Evaluation (NDE) and Nuclear Experiments".

- **NDE tasks/activities:**
  - General purpose neutron cross section evaluations (ENDF), incl. co-variances
  - Special purpose nuclear data evaluations & libraries: neutron activation, displacement damage, gas production, deuteron cross-sections
  - Methods/tools developments
  - Testing and benchmarking (V&V, S/U analyses)

Contributing research institutions: CCFE – Culham, UK; IFIN-HH – Bucharest, Romania; JSI – Ljubljana, Slovenia ; KIT – Karlsruhe, Germany; PSI - Würenlingen, Switzerland; TUW – Vienna, Austria, UNED – Madrid, Spain; UU – Uppsala, Sweden

General Purpose Nuclear Data Evaluations

Complete ENDF data files with co-variance data up to 200 MeV neutron energy

- **n + $^{180, 182, 183, 184, 186}$W** ⇒ *A. Konobeev, R037*
  - Evaluation by KIT, Germany, applying **Bayesian approach** taking into account experimental and model uncertainties.
  - Nuclear model calculations based on modified **TALYS code** for prior calculations and **GLS technique** for generation of co-variance data and updating of evaluation.
- **n + ^{56}Fe** ⇒ *G. Schnabel, R033*
  - **Trial evaluations** by PSI, Switzerland, and UU, Sweden, using **advanced evaluation methodologies**
  - **Randomly generated data files** (varying models and parameters), validation against criticality and shielding benchmarks.
  - Simulation of **model defects** based energy-dependent TALYS parameters modelled by **Gaussian Processes (GP).**
- **n + ^{16}O** ⇒ *H. Leeb, R046*
  - **Hybrid R-matrix approach** to model reaction channels in resonance region by TUW, Austria
  - Unified evaluation procedure utilizing combined prior co-variance matrix from statistical and R-Matrix regimes and GLS approach for the Bayesian updating of the evaluation.

ENDF data files include all information/data required for fusion technology applications (transport simulation, nuclear responses, uncertainties), neutron energy up to 200 MeV

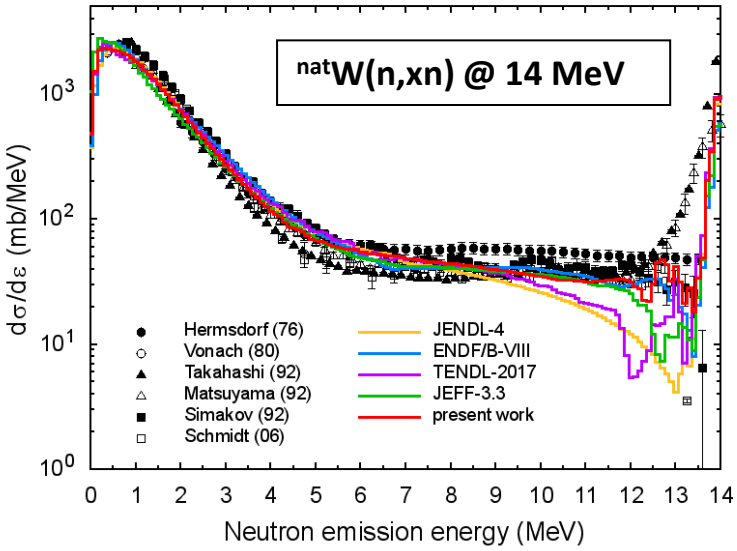
Evaluated n + $^{180, 182, 183, 184, 186}$W cross-section data

- *Nuclear model calculations: Modified TALYS code using geometry dependent hybrid (GDH) model for pre-equilibrium reactions*
- *Resonance parameters from JEFF-3.3 ($^{182, 183, 184, 186}$W) and Mughabghab (^{180}W)*
- *Generalized Least Square (GLS) technique for co-variance data generation and Bayesian updating of evaluation*

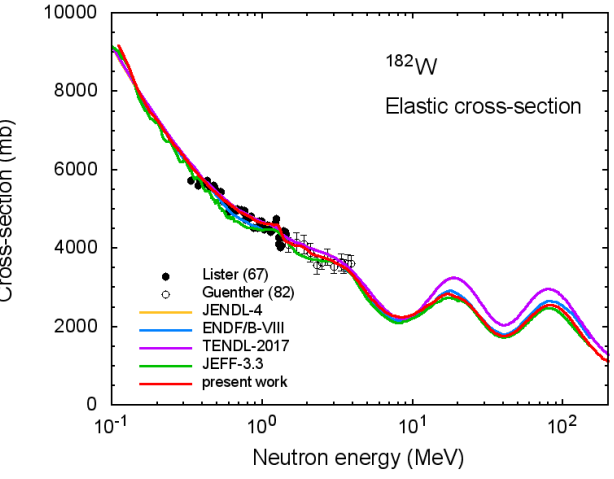
Karlsruhe Institute of Technology

⇒ *A. Konobeev, R037*

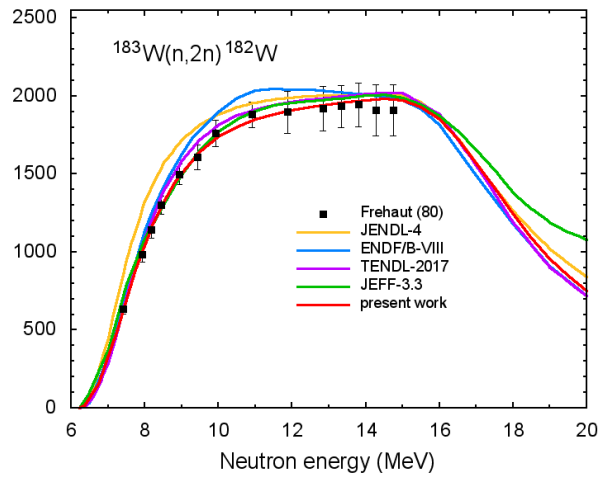
^{nat}W neutron emission cross-section



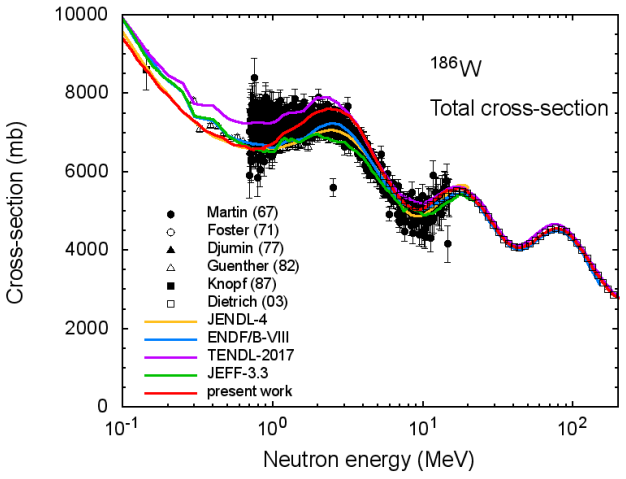
^{182}W(n,n)^{182}W



^{183}W(n,2n) ^{182}W



^{186}W total cross-section



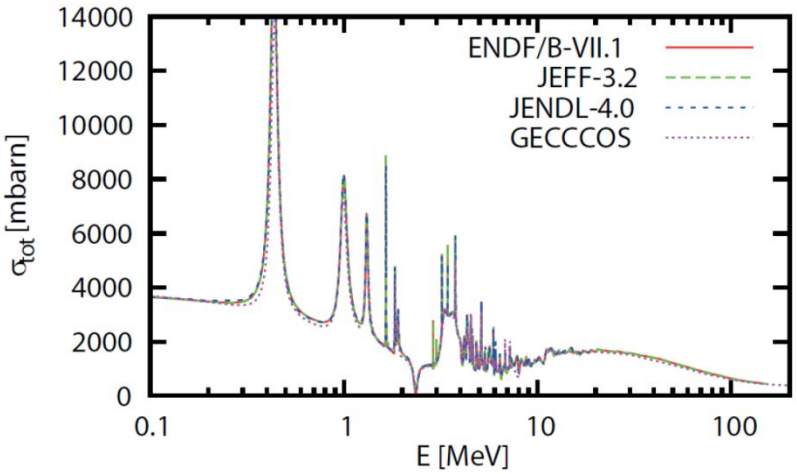
Evaluation of n + ^{16}O cross-section data using Hybrid R-Matrix approach

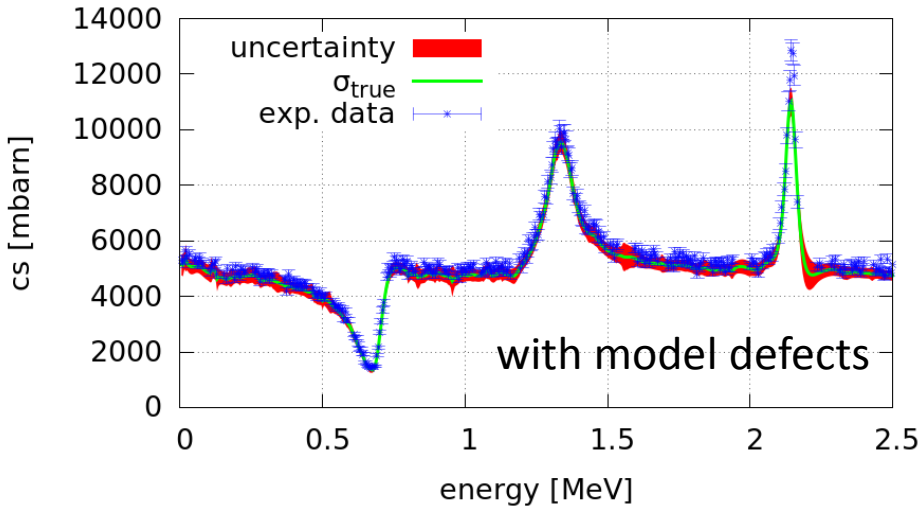
- ***Hybrid R-matrix fit*** *in energy range 1 keV – 14 MeV using TUW code system* ***GECCCOS***
- *Statistical model fit using TALYS with optimized optical potentials (1 keV – 200 MeV)*
- *Unified Bayesian evaluation* ***accounting for model defects*** *(in resonance and statistical energy range) providing co-variance matrices*

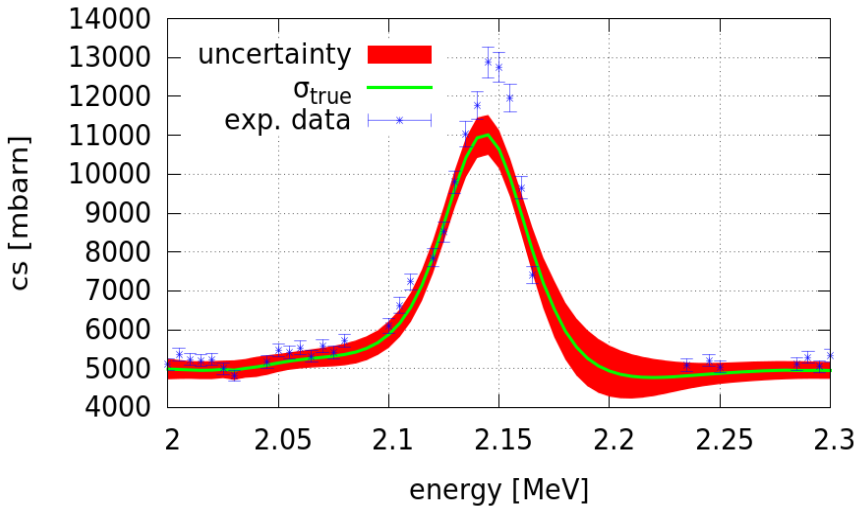
⇒ *Production of full ENDF prototype data file for use in benchmark analyses*

⇒ ***H. Leeb, R046***

Total cross-section n + ^{16}O

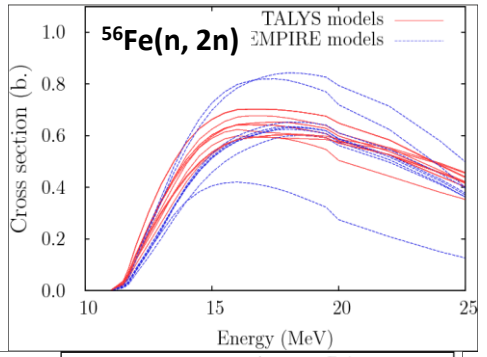


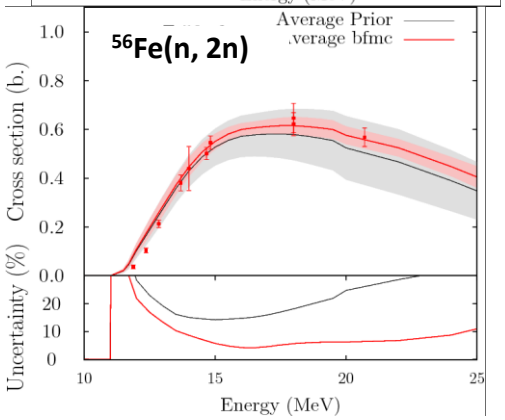




Evaluation of fast n + ^{56}Fe cross-sections using advanced evaluation methodologies

- ***Randomly generated nuclear data evaluations/files***
  - *Extension of TMC method (A. Koning, D. Rochman)*
  - *Varying nuclear models (e. g. gamma strength functions, leve densities, optical models, … from TALYS & EMPIRE) and parameters (n + ^{56}Fe: 18 000 random files created)*
  - *BMC/BFMC method to find best final evaluation*
  - *Testing with criticality and shielding benchmarks*



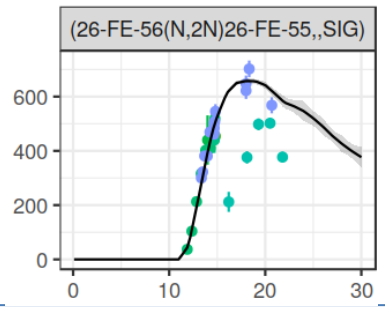


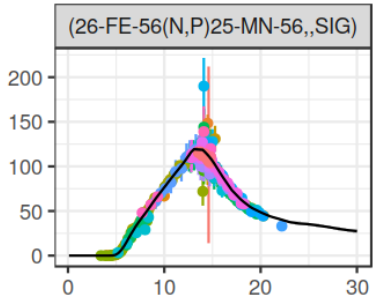
- ***Model defects to describe imperfect physical models and data inconsistencies***

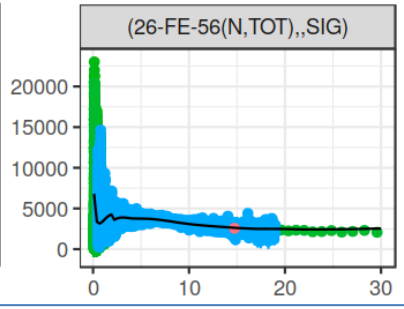
⇒ ***G. Schnabel, R033***

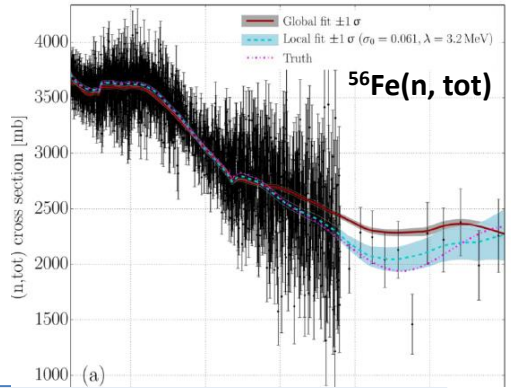
  - *Simulation of model defects by energy-dependent parameters in TALYS code*
  - *Parameter functions modelled as Gaussian processes fitted together with energy-independent parameters*

  ⇒ *Demonstration ENDF data file up to 30 MeV*







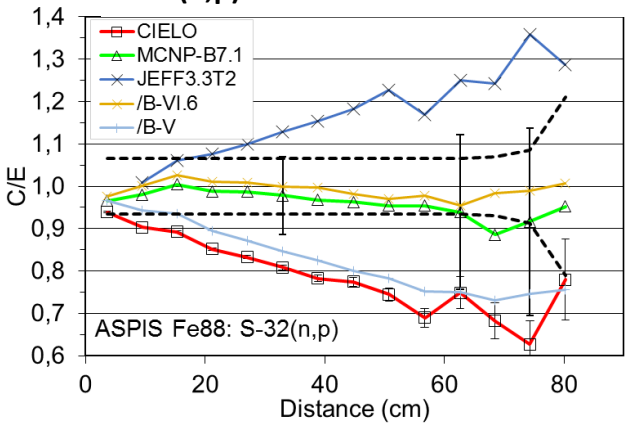


Benchmark and validation analyses

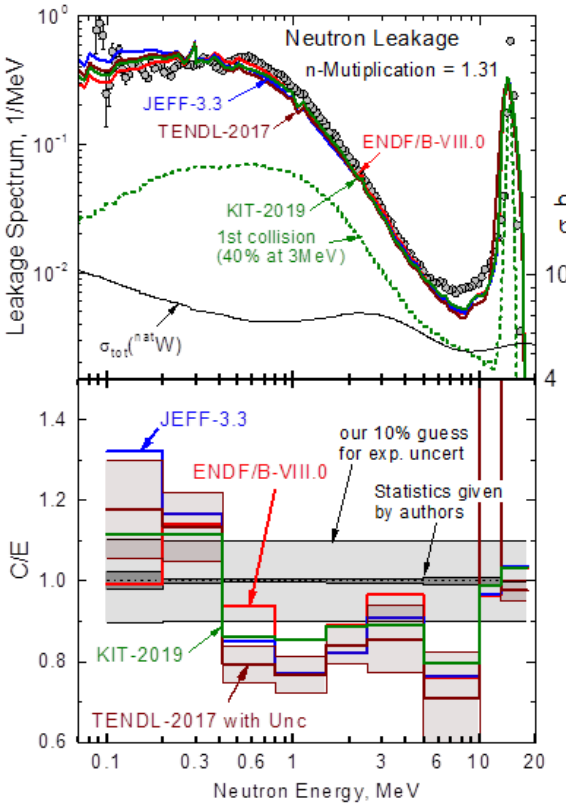
To support running general purpose evaluations and testing of specific JEFF data of major interest to fusion applications in EUROfusion/PPPT

- *Current focus on O, Fe, W: Benchmarking against FNS experiment (liquid O slab), Fe spherical shells (IPPE, KfK, NIST, Rez with 14 MeV + ^{252}Cf neutron source, ASPIS IRON-88, Oktavian spherical shell (W)*

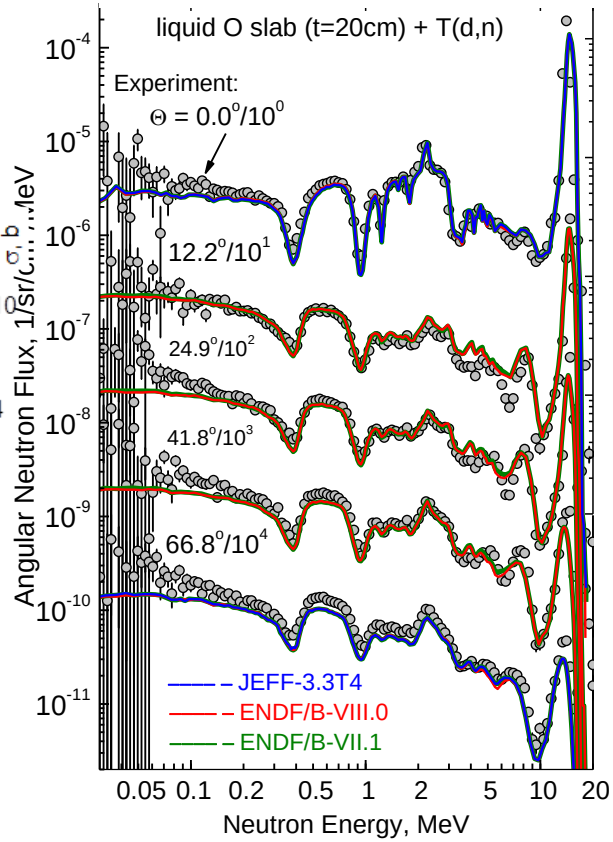
ASPIS IRON-88 benchmark experiment, S-32(n,p) reaction rate measurements



Oktavian W spherical shell (R/r= 20.15/10.2 cm), neutron leakage



FNS liquid O slab (20 cm), angular neutron leakage flux spectra



⇒ ***To be extended for running data evaluations on ^{16}O (TUW), ^{56}Fe (UU/PSI), stable W isotopes (KIT)***

Activation Cross-Section Data Library

European Activation File (EAF):

- EAF series developed by CCFE/NRG in the frame of EU fusion programme, EAF-2010 latest version (frozen, no further development)

Strategy adopted in PPPT programme: Establish TENDL as reference data library for activation calculations

- TENDL - "TALYS based Evaluated Nuclear Data Library"
  - *Developed previously by NRG, now PSI, in collaboration with IAEA, CCFE, CEA and others*
  - *Very comprehensive and complete data library, largely based on automated TALYS calculations with default and adjusted parameters and data from other source*
  - *Includes cross-section data for n, p, d, t, ^{3}He, α and γ induced nuclear reactions*

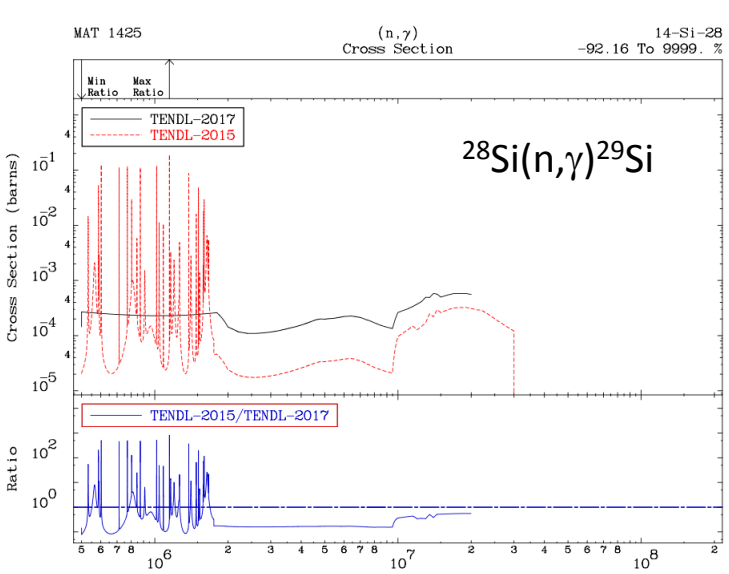
$\Rightarrow$ TENDL to preserve or increase quality of EAF-2010 for activation calculations by including validated cross-sections and removing observed deficiencies

- Deficient cross-sections identified and prioritised according to needs of fusion programme (DEMO, IFMIF-DONES, ITER) improved and included in TENDL-2017

$\Rightarrow$ *Dedicated Activation Data File ("EAF format") produced from TENDL-2017, adopted as JEFF-3.3 activation data library ,*

$\Rightarrow$ *211 group data library to be adopted as reference for PPPT programme (after successful completion of V&V analyses), superseding EAF-2010.*

Improved Activation Cross-Sections in TENDL-2017



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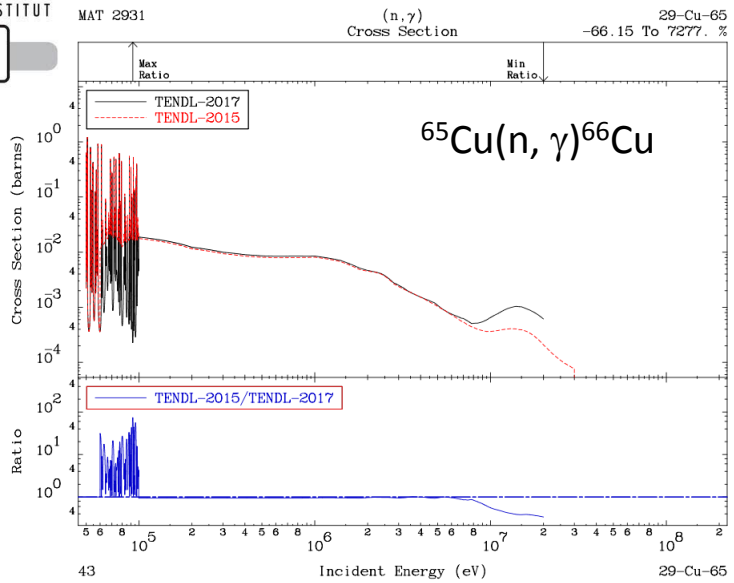
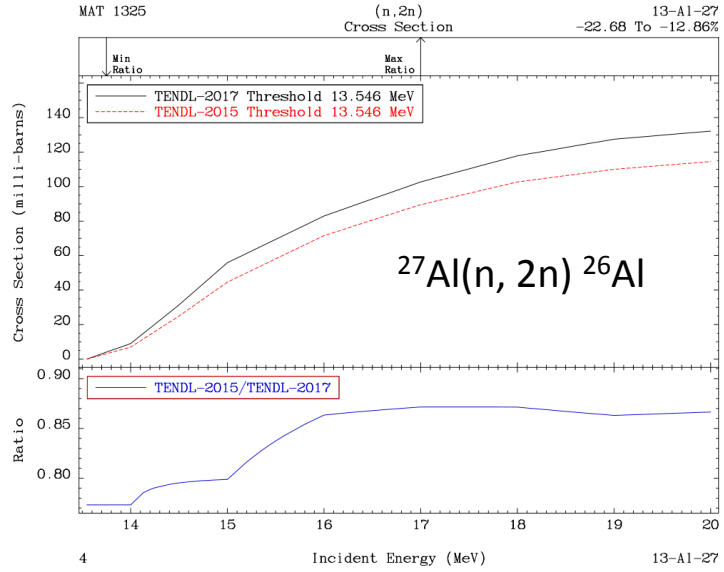
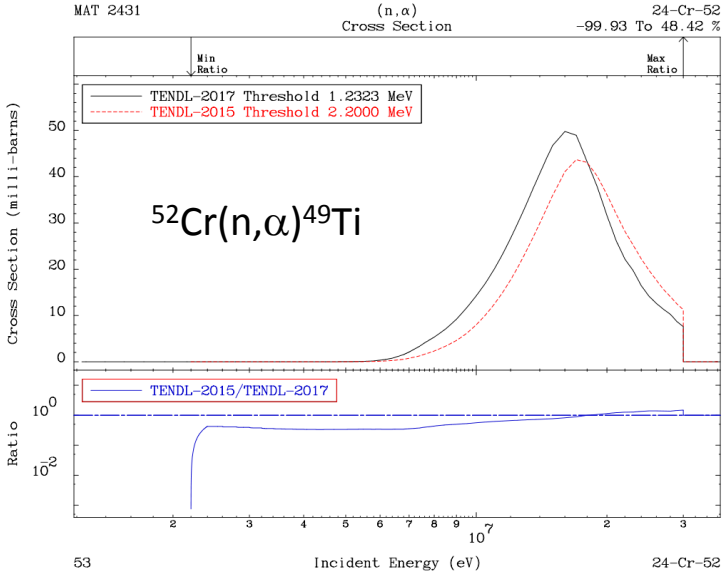






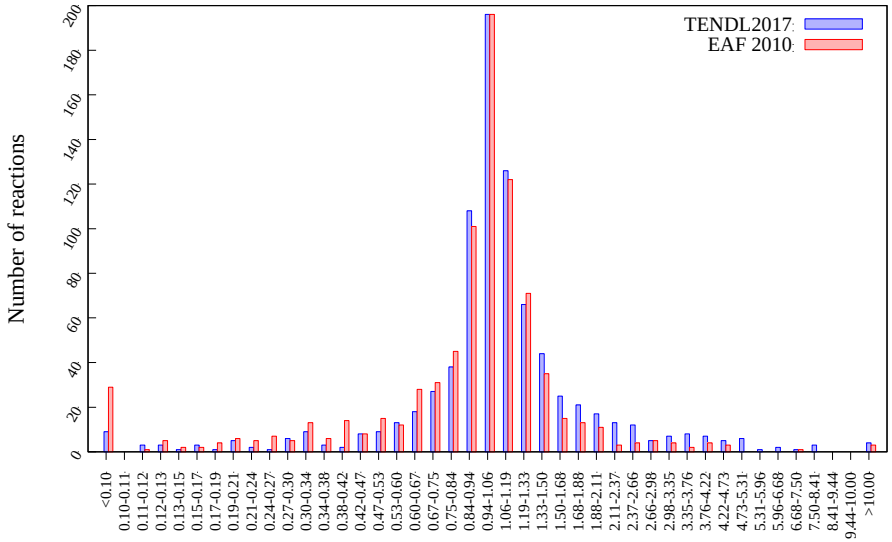
Validation of TENDL-2017 Activation Cross-Sections

V&V analyses for range of integral measurements in fusion/accelerator systems, decay heat simulations, MACS and statistical checks using CCFE validation data base

CCFE
CULHAM CENTRE FOR FUSION ENERGY

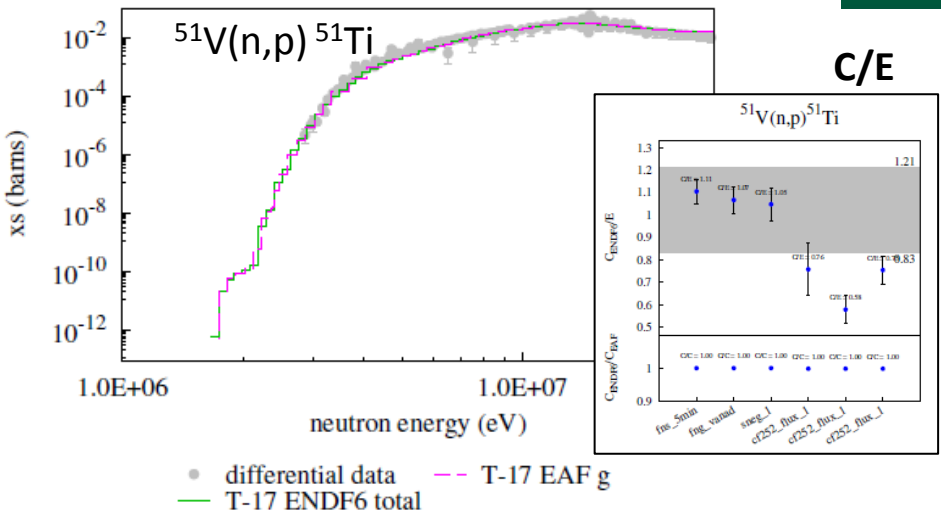
UNED

TENDL-2017 (709 groups, ENDF format)



C/E ratios for all integral measurements

TENDL-2017 (211 groups, EAF format)



TENDL-2017 ENDF/709g vs. EAF/211g:

- *Overall good agreement, except for (n,t) and (n,h) reactions*
- *Minor effects due to different group structures*
- *Some inconsistent data identified (low mass nuclides) and fixed, V&V running*

Conclusion:

- *TENDL-2017 provides superior agreement with experimental data*
- *Recommended as basis for activation data library in fusion applications*

α-particle Optical Model Potential (OMP)

Improved OMP for α-particle emission in neutron induced reactions

⇒ *V. Avrigeanu, R022*

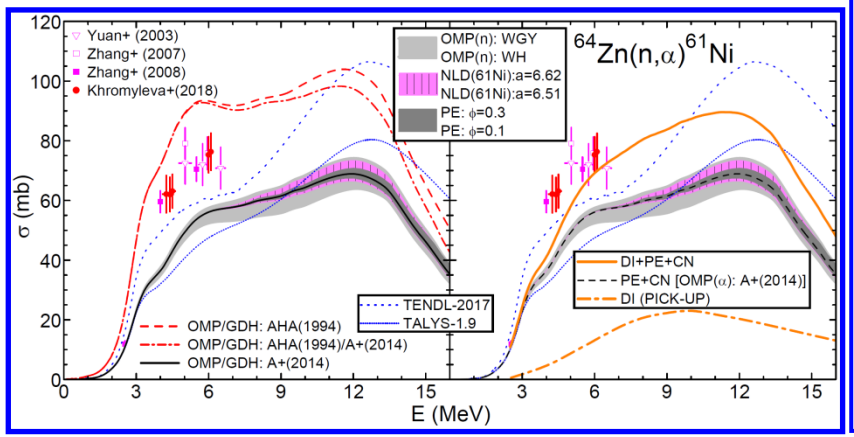
- OMP elaborated previously (M.+V. Avrigeanu), implemented as default option in TALYS 1.9.

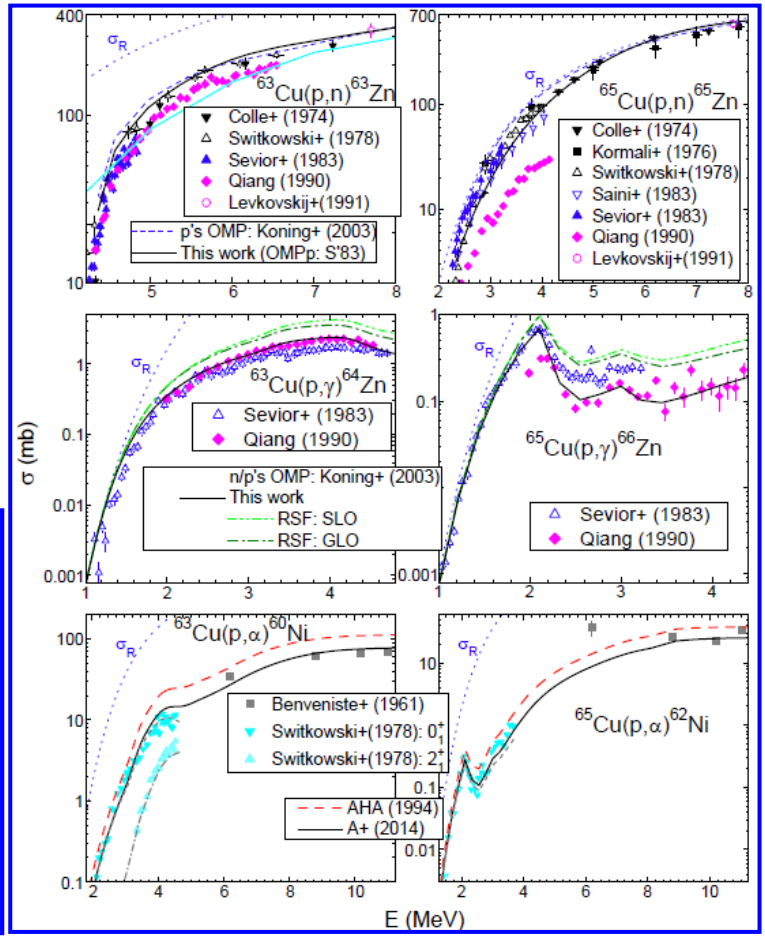
⇒ *Continued studies to further improve α-emission data on the basis of consistent nuclear model calculations*

⇒ *Including low energy proton data to understand open questions in α-particle OMP*

⇒ *Taking into account all available data for reaction channels and isotopes of Eurofer and SS-316 steels*

n/p induced α-emission on Zn/Cu -> Ni



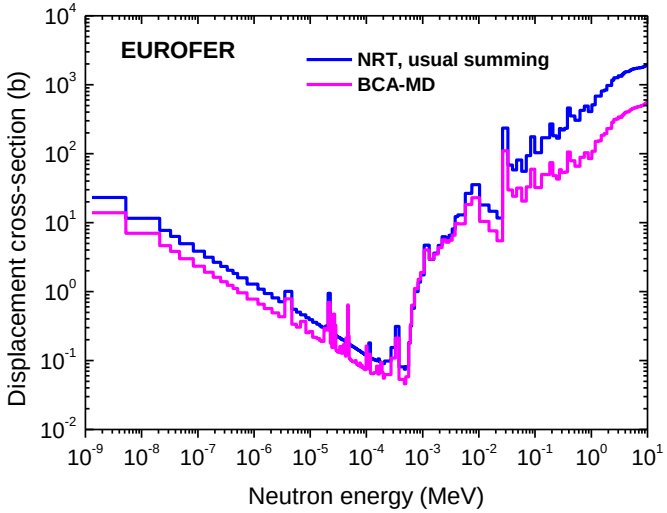


Displacement Damage Cross-Section Data

Dedicated displacement damage cross-section data for major steels used in DEMO and IFMIF-DONES as structural materials: Eurofer (low activation) and SS-316

- **Advanced DPA cross-section data** up to 150 MeV for steel constituents based on atomistic modelling approach.
  - *Molecular Dynamics (MD) and Binary Collision Approximation (BCA) model simulations for the calculation of number of lattice defects*

  ⇒ *Better agreement with experimental point defect production data.*



- Displacement damage cross-sections available through IAEA/NDS:

  Eurofer: https://www-nds.iaea.org/public/download-endf/DXS/EUROFER_dpa-XS/ACE

  SS-316: https://www-nds.iaea.org/public/download-endf/DXS/SS-316_dpa-XS/ACE/

  ⇒ *Provided as ACE data files for use with MCNP as dosimetry cross-sections*

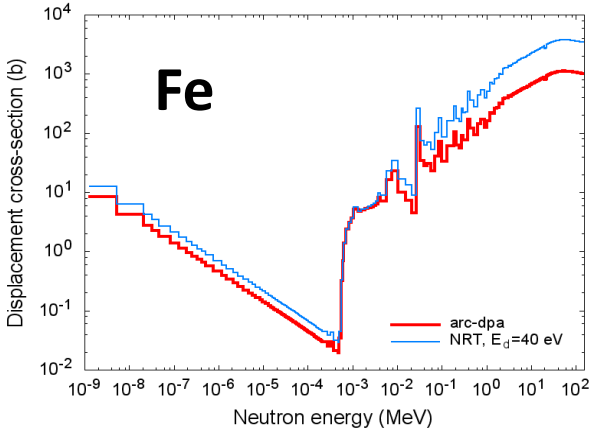
  ⇒ *Recommended for use in PPPT neutronics ("Guidelines for for Neutronic Analyses")*

Displacement Damage Cross-Section Library

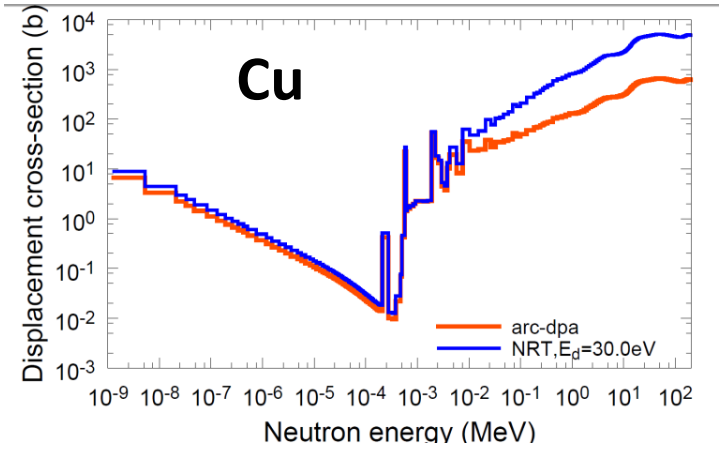
DPA cross-section data library for individual elements

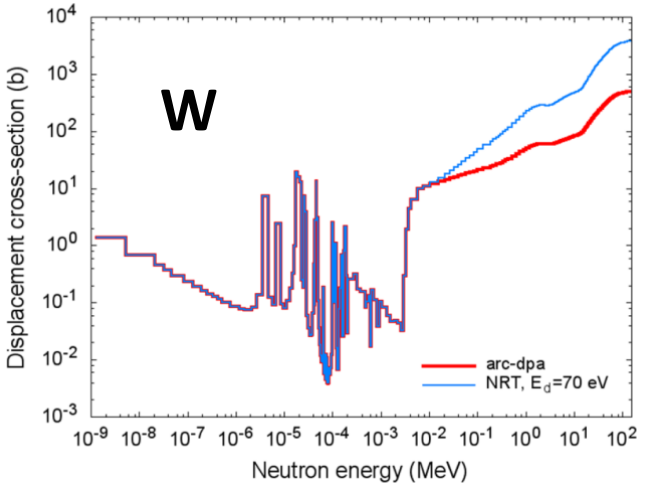
- Complete data library for elements Li to U up to 200 MeV neutron energy based on JEFF-3.3 neutron cross-section data (A. Konobeev, KIT)
- DPA cross sections prepared with standard **NRT damage model** and **Arc** [*] ("athermal recombination corrected") **dpa approach** to take into account lattice defects surviving thermal annealing.
- Provided as JEFF-3.3 sub-library by the NEA Data Bank:

  http://www.oecd-nea.org/dbdata/jeff/jeff33/#dpa



Arc dpa vs NRT dpa



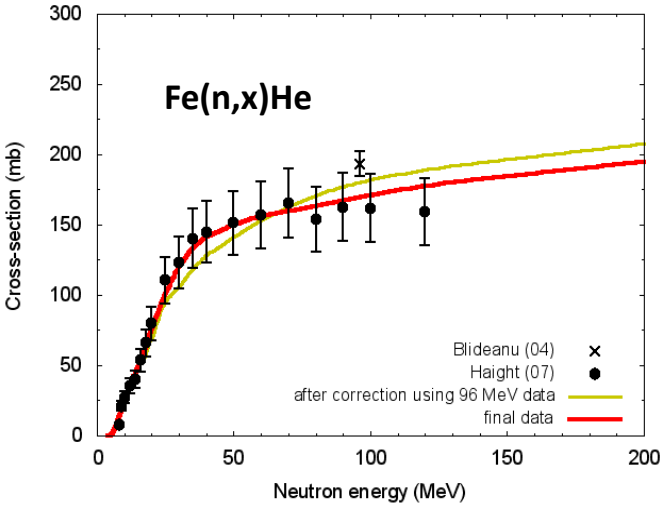


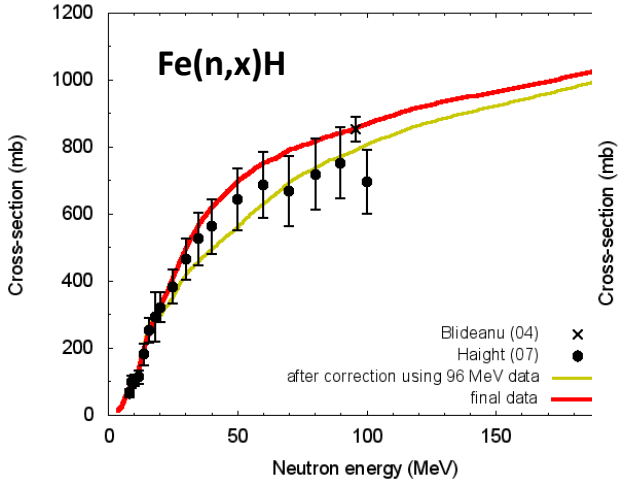
[*] *K. Nordlund et al., NEA/NSC/DOC(2015)9, OECD 2015*

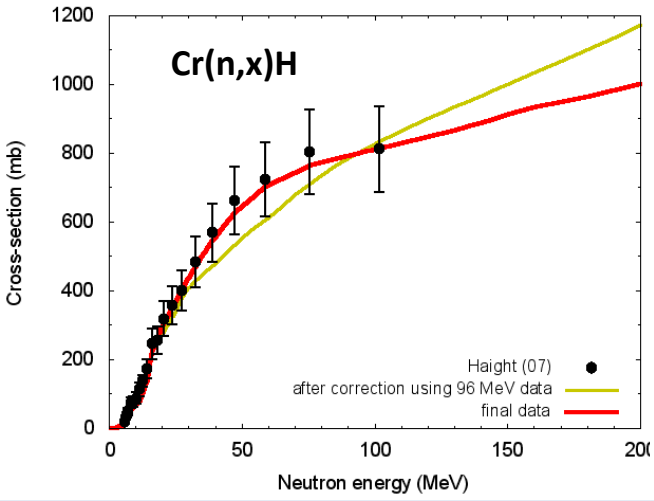
Gas Production Data Library

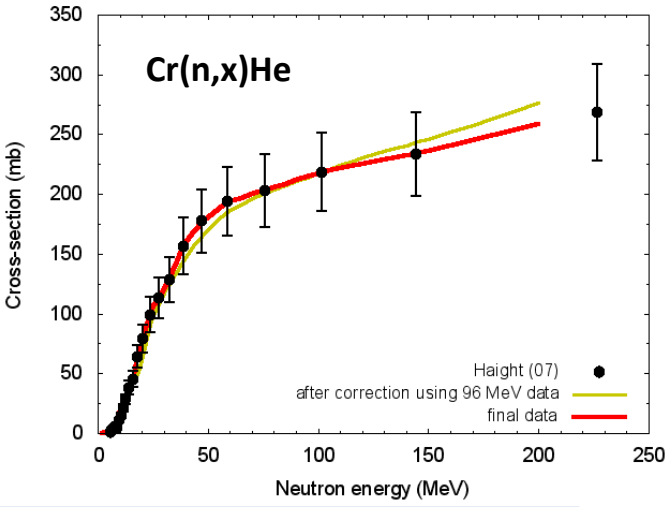
Gas production important for material performance (DEMO, IFMIF-DONES)

- Systematically evaluated gas production cross-sections for nuclides Z=12 to 83 up to 200 MeV neutron energy
  - *Based on experimental data, evaluated data, nuclear model calculations and systematics, and statistical combination of experimental and theoretical data*
  - *Includes production of protons, deuterons, tritons, ^{3}He, and α-particles in neutron induced reactions on 262 stable nuclides*
- Data available at: https://www.inr.kit.edu/img/gas_production_files.zip





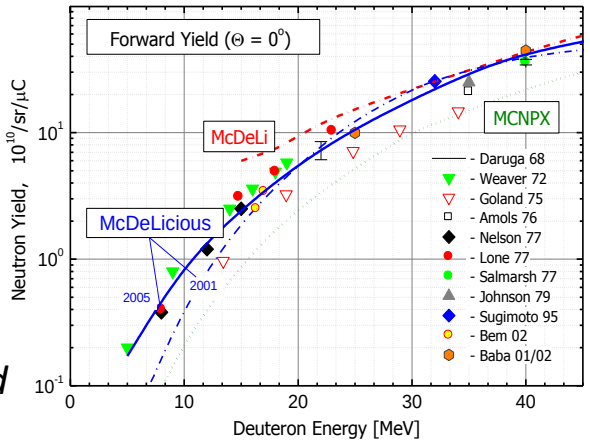


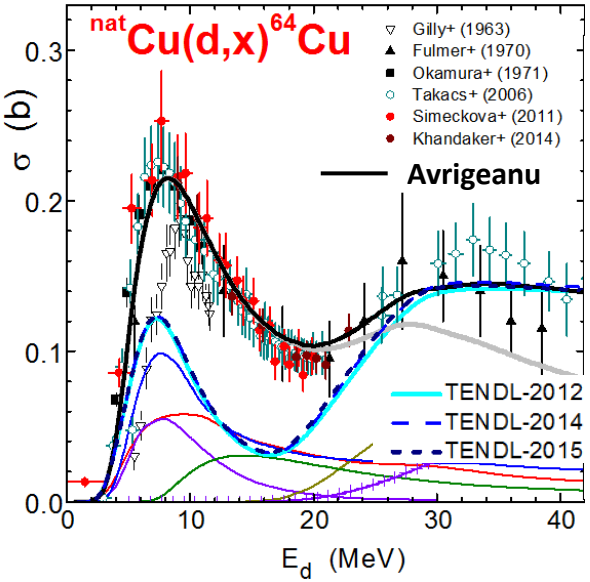


Deuteron Induced Cross-Section Data

Required for IFMIF-DONES neutron source facility – ENS (Early Neutron Source) project in PPPT programme

- Neutron generation in Li target: ^{6,7}Li(d, xn) cross-section data provided with McDeLicious MC code, validated with measured thin and thick target yield data
- Deuteron cross – section data for activation calculations:
  - ⇒ *Available with TENDL data library, largely based on automated TALYS calculations with default model and parameters lacking sufficient accuracy*
  - ⇒ ***Dedicated effort in PPPT programme to improve nuclear models describing deuteron induced reaction mechanisms***
- Deuteron cross – section data for transport simulations:
  - ⇒ *Available with the same TENDL deuteron data library*
  - ⇒ *Can be used in deuteron transport simulations with MC code code MCUNED (P. Sauvan, UNED) and MCNP-6.*
  - ⇒ *In general, poor data quality because of deficient reaction models in TALYS, to be improved in PPPT programme !*





Deuteron Induced Cross-Section Data

Dedicated evaluation effort to improve deuteron cross-section data for transport simulations and activation calculations

⇒ *M. Avrigeanu, R016*

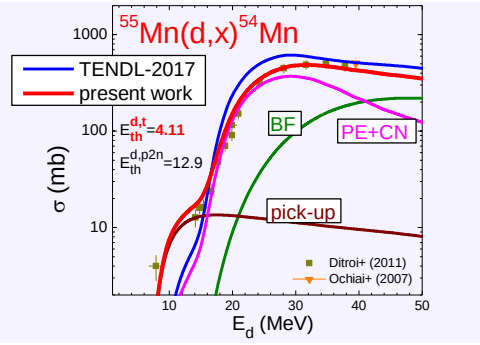
- Advanced modelling approach taking into accounted deuteron break-up, stripping, pick-up, pre-equilibrium and evaporation processes

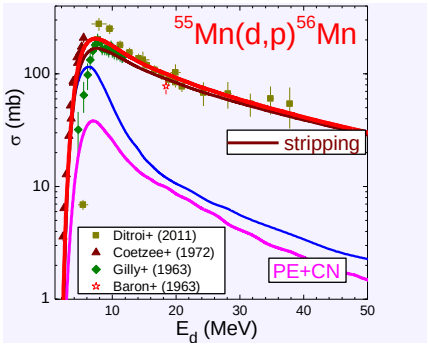
  ⇒ *Implemented in ad-hoc modified TALYS version 1.81*

- Evaluation of d-induced reaction cross-sections for ^{27}Al, **$^{50, 52, 53, 54}$Cr**, **^{55}Mn**, ^{54,56,57,58}Fe, ^{58,60,61,62,64}Ni, ^{63,65}Cu, ^{93}Nb up to 60 deuteron energy MeV

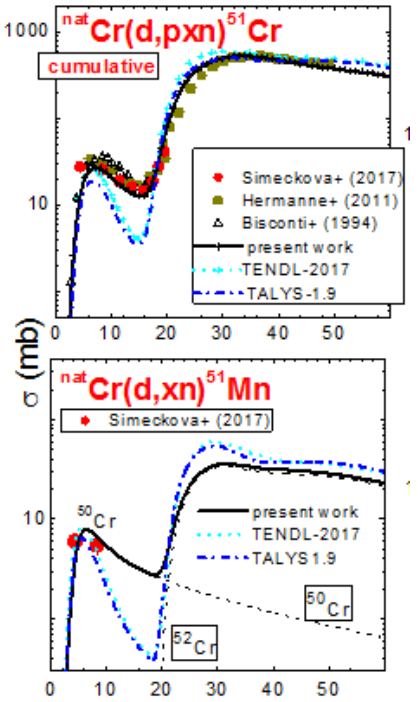
  ⇒ *Very good agreement with experimental data*

d + ^{55}Mn cross-sections (ongoing evaluation)





d + ^{nat}Cr cross-sections



⇒ *Improved cross-sections to be included in new TENDL deuteron data library, extended to other nuclides & reactions*

Deuteron Induced Cross-Section Data

Complementary approach to improve use of evalutaed deuteron cross-section data in transport simulations

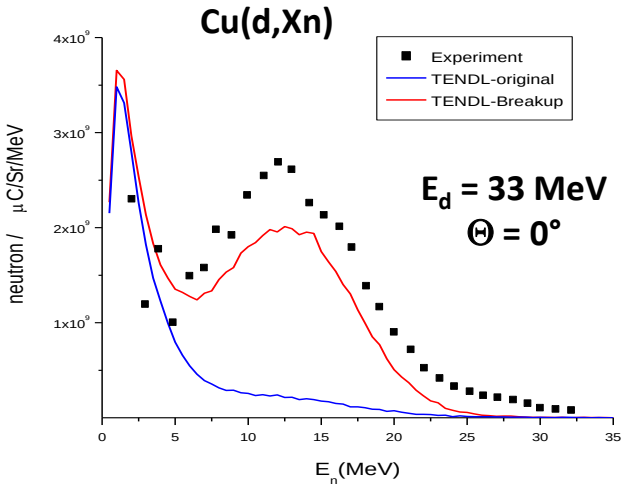
- MCUNED code (P. Suavan, UNED): Parameterised representation of deuteron break-up
- Based on recent Kalbach-Mann formalism to describe angular distributions of secondary particles emitted in deuteron break-up reactions

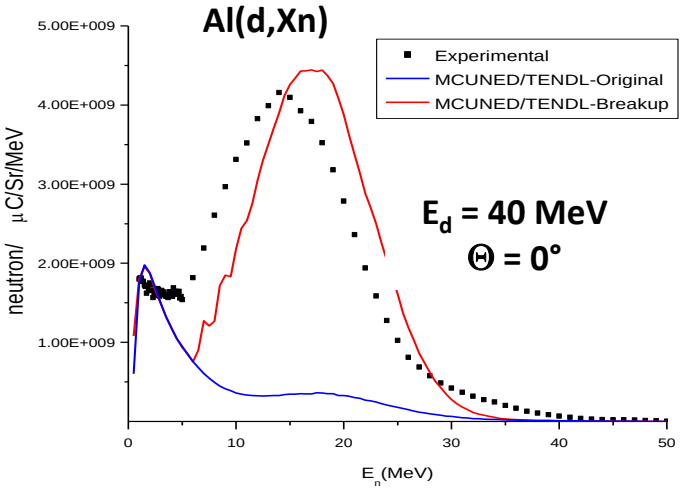
⇒ *Requires format modification on ENDF data file*

⇒ *Successfully tested with ad-hoc modified TENDL deuteron data library*.

P. Sauvan, A. Koning, F. Ogando, J. Sanz, "Implementation of a new energy-angular distribution of particles emitted by deuteron induced nuclear reaction in transport simulations", EPJ Web of Conferences 146, 02010 (2017)

⇒ *Option considered for representing deuteron cross-sections in TENDL deuteron data library for use with MCUNED code (not MCNP.6)*





Summary & outlook

- **Nuclear data for fusion technology**
  - *High quality data essential for design optimization, performance evaluation; safety, maintenance and waste management*

  ⇒ *Pre-requisite to ensure reliable analyses and results*

- **Dedicated development efforts in PPPT/EUROfusion**
  - Tailored to PPPT project needs: DEMO, IFMIF-DONES
  - Activities coordinated/aligned with JEFF

  ⇒ *Nuclear data for transport simulations – neutrons, deuterons*

  ⇒ *Activation cross-section data - neutrons, deuterons*

  ⇒ *Special purpose data, e. g. displacement damage, gas production*

- **Supporting experimental activities**
  - *Benchmark experiments: neutron transport/shielding, breeding, activation*
  - *Cross-section measurements (high energy range): activation, gas production, dosimetry, …. displacement damage , ….*

  ⇒ *New in PPPT/EUROfusion (2019): WCLL breeding blanket mock-up experiment & complementary activities related to gas production and damage cross-sections.*