

The predictive power of TALYS

Arjan Koning

Nuclear Data Section International Atomic Energy Agency, Vienna

Workshop for Applied Nuclear Data Activities (WANDA 2021) Session One: Predictive codes for Isotope Production 25 Jan - 3 Feb 2021, USA (Video Meeting)

TALYS: An attempt to streamline all important 60 Years nuclear (reaction) physics into one code scheme

- Used for fundamental nuclear physics research
- Produces nuclear data for applications
- <u>www.talys.eu</u>



Domain of TALYS

- Projectiles: neutron, photon, proton, deuteron, triton, Helium-3, alpha particle
- Targets: Z= 3-124, A=5-339
 - Reliability: Z > 6, A > 12
- Incident energy: 1 meV 1 GeV
 - Reliability: few keV 200 MeV
- 400 keywords for models, parameters, etc. **Range of TALYS**
 - (Almost) every nuclear reaction observable
 - TENDL library

Use of TALYS



TALYS principles



We insist:

- Flawless and trivial software installation
- Complete and readable manual
- **Reproducibility**: you get the same results as we show, good or bad
- A large and diverse validation set
- TALYS does not crash

We aim:

- Physics as good as reasonably possible
- Adopting your innovations in our implementation: we are a few years behind the latest and greatest developments in nuclear physics

This enables:

- Thousands of analyses of experiments
- TALYS Evaluated Nuclear Data Library (TENDL)
- Total Monte Carlo (TMC) uncertainty quantification
- ...and much more

Global predictive power of TALYS

Based on all EXFOR cross sections, A-independent



Essential 1: Optical model potential (OMP) for proton reaction cross sections

Predictive power for KD03 global proton OMP up to 200 MeV ~ 8%

Essential 2: Nuclear level densities

Different level density models may give differences of 10-15% in peak values of excitation functions

Essential 3: **Pre-equilibrium nuclear models** (and multiple pre-equilibrium models above 30-40 MeV)

TALYS exciton model parameterisation has been established from single- and double-diff emission spectra, not from production cross sections

(See M.B. Fox et al, Investigating High-Energy Proton-Induced Reactions on Spherical Nuclei: Implications for the Pre-Equilibrium Exciton Model, Phys Rev C, tbp 2021)



Three levels of nuclear data libraries

- No experimental data: global nuclear model calculations (TALYS/TENDL)
- Some experimental data: nuclear model calculations with adjusted input parameters (TALYS/TENDL)
- Many experimental data: Generalized-Least-Squares/Pade approximation, nuclear models not needed (IAEA medical isotope library)

Essential: Complete and good/reasonable quality cross section data

TENDL: TALYS Evaluated Nuclear Data Library

- Produced by TALYS nuclear model code + other sources
- Complete in projectile (n, g, p, d, t, h, a), target (2813 nuclides) and energy range (0-200 MeV)
- 1000-1500 citations, current version TENDL-2019
- Globally reasonable predictive power....not enough!!
 Plan: Medical isotope data library combine the best with the most complete



Typical example #1: direct good fit!





Plots for all particles, all nuclides, all reactions: nds.iaea.org/talys

Typical example #2: further TALYS adjustment needed



Some final remarks



- (Multiple) pre-equilibrium models and level densities have an important impact on predictive power of model codes for isotope production.
- The predictive power of TALYS is numerically established for incident neutrons, charged particles and photonuclear to follow.
- Efficient and trivial access to **all** experimental data is essential, WPEC SG50 on curated experimental database based on EXFOR (Lewis, Neudecker) is incredibly important for TALYS development.
- There is more relevant exp. data below 40 MeV than above 40 MeV, the latter is important for various exotic routes (e.g. Ac-225 production)
- A complete nuclear data for all particles, isotopes and energies is available, TENDL, but the quality is not yet sufficient. Needed:
 - Nuclide-by-nuclideTALYS parameter adjustment
 - Evaluators who can distinguish good from bad experimental data
 - Model defect approaches (Gaussian processes etc.) for when TALYS is not sufficient



Thank you!

