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# Covariances from model variation: Application to quantities for astrophysics

*Dimitri* Rochman[1,*], *Arjan* Koning[2,**], and *Stéphane* Goriely[3,***]

[1]Reactor Physics and Thermal Hydraulic Laboratory, Paul Scherrer Institut, Villigen, Switzerland
[2]Nuclear Data Section, International Atomic Energy Agency, Vienna, Austria
[3]Institut d'Astronomie et d'Astrophysique, Université Libre de Bruxelles Brussels, Belgium

**Abstract.** In this work, covariance matrices coming from model variations, in contrast to the usual parameter variations, are presented. The considered phenomenological and microscopic models are included in the code TALYS, and concern level densities, gamma strength functions, optical potentials and masses. A total of 288 model sets for each isotope is used to estimate both uncertainties and correlations from systematical origin. The calculated quantities are of interest for astrophysical applications, such as capture cross sections, and reaction rates. The isotopes ($3 \leq Z \leq 100$) are from the proton to neutron drip lines, covering about 8800 cases, and are included in the TENDL-2021 library.

## 1 Introduction

Covariance matrices are nowadays included in almost all nuclear data libraries. They mostly concern neutron-induced reactions [1, 2], with some addition of charged particles [3]. Such matrices are useful for a number of applications, ranging from nuclear energy production to astrophysics, with also utilization for medical isotopes [4–6].

The method of assessment of such covariance matrices is based on (1) estimation of experimental uncertainties and correlations, (2) estimation of theoretical uncertainties and correlations, and (3) combination of (1) and (2). In some cases, only (1) or only (2) is used, for instance when no experimental data exists, or if theoretical values are not needed. For the theoretical estimation, almost all covariance evaluations rely on the following approach: selection of a set of preferred models, adjustment of model parameters to reproduce experimental data (or simple use of values from systematics), and then vary those parameters within acceptable ranges to produce a set of varied calculations, later used to build covariance matrices.

Such methods are well justified when the reaction models are within their range of applicability, as for stable isotopes, or isotopes "*not too far*" from the stability line. For the majority of applications related to energy production and medical isotopes, the use of such covariance matrices from libraries is therefore reasonable. In the case of astrophysics, as a large number of relevant isotopes are far from the stability line, covariance matrices as presented in the TENDL libraries (for isotopes with half-lives as short as 1 second) might be less justified: the main reason is that most of the theoretical reaction models are not proven to be correct for exotic nuclei and model uncertainties are known to dominate over parameter uncertainties (see for instance Refs. [7, 8]). A number of examples can also be found in Refs. [9, 10] for the impact of various gamma-ray strength functions.

An alternative approach to the estimation of covariance matrices is proposed here, by varying reaction models and not model parameters. For instance, a capture cross section might differ with different level density models, or with different gamma-ray strength functions. Such changes can be used to assess systematical changes in cross section calculations. A similar approach was presented in Ref. [11] for the proton-induced reactions on $^{59}$Co where the goal was to provide the most appropriate set of models and their parameters. All cross sections and covariance matrices were affected by the variation of models.

Details of the methods and examples are presented in the following, based on TALYS calculations applied to capture cross sections and Maxwellian Averaged (n,$\gamma$) Cross Sections (or MACS). A large number of nuclei are considered ($3 \leq Z \leq 100$), from the proton to neutron drip lines, representing about 8800 isotopes. As presented in the following, these models were not validated for such number of isotopes, and the goal of this work is to assess the impact of the available models. Quantities for nuclear reactions are currently used in astrophysics for very exotic isotopes, often based on a single choice of models. The current work will help to recognize the impact of reaction models. Most of the present results are included in the TENDL-2021 nuclear data libraries.

## 2 Model variation

The method applied here is conceptually relatively simple: perform different TALYS calculations with different

*e-mail: dimitri-alexandre.rochman@psi.ch
**e-mail: a.koning@iaea.org
***e-mail: stephane.goriely@ulb.be

input models, and compare calculated quantities. The outcome of such calculations is an estimation of changes due to model selections. Compared to the traditional approach of selecting one set of models and changing model parameters, an estimation of systematical effects can be performed.

In practice, the following models are considered (as implemented in TALYS):

- E1 gamma strength functions with two possibilities (TALYS keyword *strength* with values 8 or 9 ): either Gogny D1M HFB+QRPA, or SMLO.
- Level density (TALYS keyword *ldmodel* with values 1, 2 or 5): Constant temperature + Fermi gas model, or Back-shifted Fermi gas model, or Microscopic HFB with combinatorial model.
- Optical model potential (TALYS keyword *jlmomp* with values y or n): JLM microscopic optical model potential or KD optical model.
- Gamma strength function for M1 (TALYS keyword *strengthM1* with values 3 or 8): SMLO or Gogny D1M HFB+QRPA,
- Collective enhancement for level density (TALYS keyword *colenhance* with values y or n): yes or no,
- Width fluctuation (TALYS keyword *widthmode* with values 0, 1 or 2): no width fluctuation, Moldauer model, or Hofmann-Richert-Tepel-Weidenmueller model,
- Mass model (TALYS keyword *massmodel* with values 0, 1, 2 or 3): Duflo-Zuker formula, FRDM 2012 table, Skyrme-HFB table, or D1M Gogny-HFB table (except for known masses, where the experimental value is always used)

In total, one can combine the variation of 7 model categories; in the following, specific combinations of models are indicated with 7 digits, such as 91n3n12 (default TALYS choice), or 81n8n12. Not all combinations are considered: for instance the microscopic gamma-ray strength model (*strength=8*) is only used with *strengthM1=8* for consistency. Similarly, the collective enhancement of the level density is disabled with the microscopic level density (*ldmodel=5*). In total, 288 combinations of models are used.

Among these 288 combinations, model parameters were adjusted to fit the experimental capture cross sections in the fast energy range for 12 model combinations: 91n3n12, 81n8n12, 81n8y12, 91n3y12, 95n3n12, 95n3y12, 85n8n12, 85n8y12, 82n8n12, 82n8y12, 92n3n12 and 92n3y12. It means that for these model sets, the agreement between calculated and measured neutron capture cross sections is expected to be excellent, within typically 10 %. When no experimental data exist, the parameters of these model sets will be based on non adjusted values.

## 3 Examples

Many examples can be extracted from the large amount of calculated quantities. A short selection is presented below to illustrate the content of the TENDL-2021 database for astrophysics applications.

### 3.1 Tin neutron-capture cross sections

To illustrate the variation of cross sections from stable isotopes to exotic ones, Fig. 1 presents the variation of neutron-capture cross sections for two Sn isotopes: $^{120}$Sn and $^{160}$Sn. For each of them, 288 TALYS calculations are performed, leading to 288 different cross sections per isotope. The 12 selected models are indicated as “Best models” and the other 276 as “Other models”. It can be observed that in the case of the stable isotope $^{120}$Sn, the variations are smaller than for the very exotic one. In the case of $^{160}$Sn, the capture cross section is small enough to be out of the range of the plot. Naturally, uncertainties and correlations will strongly differ between these two isotopes. If only model parameters for a selected set of models were varied (for instance for the default TALYS models 91n3n12), then such strong effect would not appear. For $^{120}$Sn, the uncertainties due to the variation of model parameters for 91n3n12 (called TENDL in the figure) are significantly smaller than the spread of all capture cross sections from model variations. The effect on this stable isotope is not as dramatic as for $^{160}$Sn. Correlations also strongly changed between both approaches, as presented in Figs. 2 and 3.

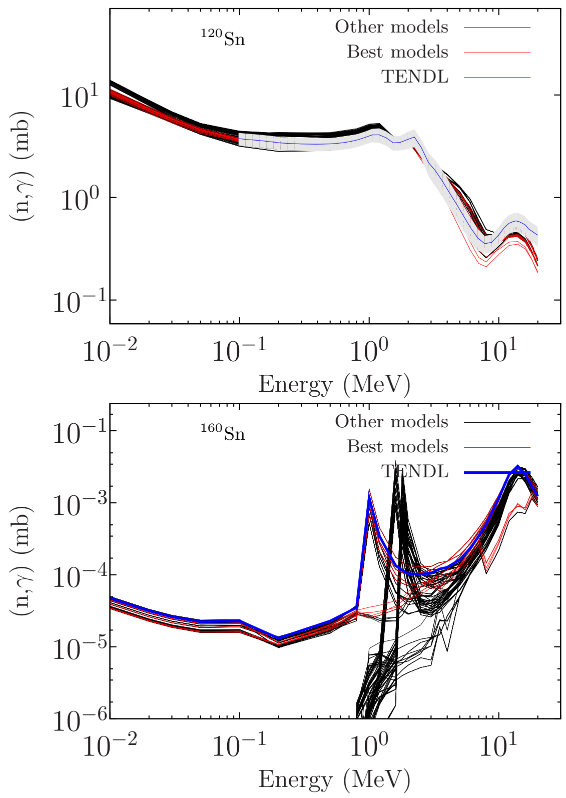



Figure 1: Example of radiative neutron-capture cross sections for two Sn isotopes (from top to bottom: 120 and 160). For each mass, 288 TALYS calculations are presented, based on different model sets.

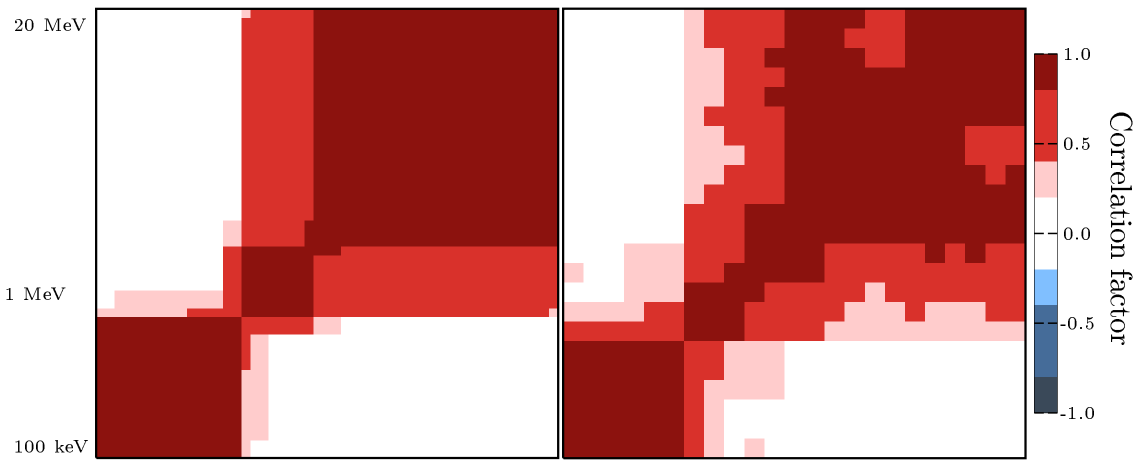



Figure 2: Correlation matrices for $^{120}$Sn based on variation of model parameters (left) and models (right)

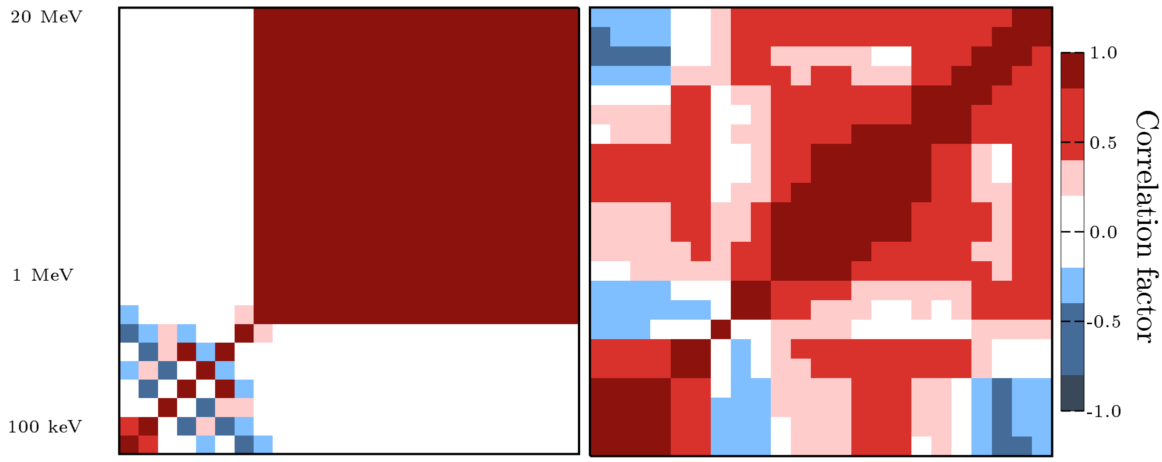



Figure 3: Same as Fig. 2, but for $^{160}$Sn.

In these figures, the X- and Y-axis correspond to the incident neutron energy. For $^{120}$Sn, the correlation matrix is not strongly modified between both approaches, as all calculated capture cross sections are very similar. Varying models lead to more degrees of freedom for exotic nuclei: for $^{160}$Sn, correlations are strongly modified, due to more pronounced changes in cross sections.
These examples illustrate the effect of varying models; additionally, these examples show that uncertainties and correlations always depend on the underlying modeling assumptions.

### 3.2 30 keV neutron-capture cross sections

As an additional example, the ratio of the neutron capture cross section at 30 keV from the default TALYS models (91n3n12) over the model set 81n8n12 is presented in Fig. 4 for all the 8800 isotopes. Clearly, strong differences can be observed for exotic nuclei. As parameters for both model sets were adjusted for stable isotopes, differences are not pronounced in the stability valley. Following this approach, all model sets can be used to calculate quantities of interest for astrophysics, such as neutron capture cross sections from 0.01 eV to 20 MeV (available from the TALYS output file called *xs000000.tot*), neutron capture reaction rates for all temperatures of astrophysics relevance taking into account the thermal population of the target (from the TALYS file *astrorate.g*), the normalized partition function G(T) (from the TALYS file *astrorate.tot*) and the Laboratory (not stellar) MACS (from the TALYS file *macs.g*).

### 3.3 Cross isotope correlations

All the quantities presented in this work are obtained with the same approach, identical calculations and model sets. Because of these similarities, correlations among isotopes for any calculated quantities can be expected. An example is presented in the following for the MACS quantity at the neutron energy of 30 keV. For each isotope, uncertainties from the variation of models can be obtained (these values can be found in the TENDL-2021 database). Additionally, as the same 288 models are used for all isotopes, correlations among isotopes can also be calculated for the MACS, as well as for other quantities. The correlation matrix in this case is presented in Fig. 5. In this figure, the

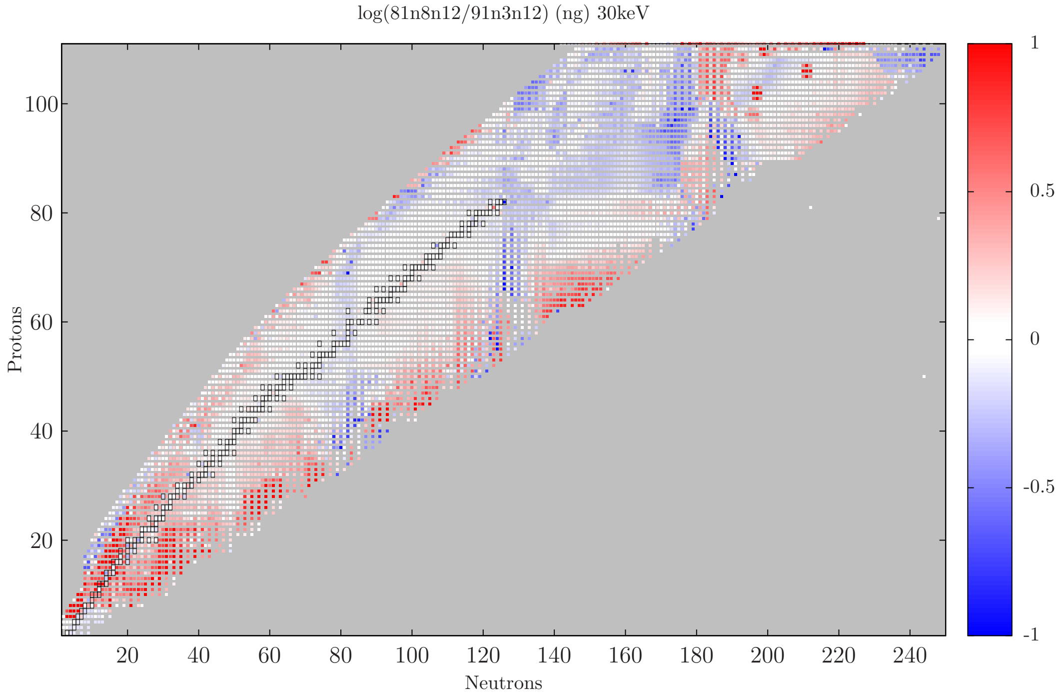



Figure 4: Ratios of model set 81n8n12 over the default TALYS model set 91n3n12 for the neutron capture cross sections at 30 keV. The color scale is the log of the ratio.

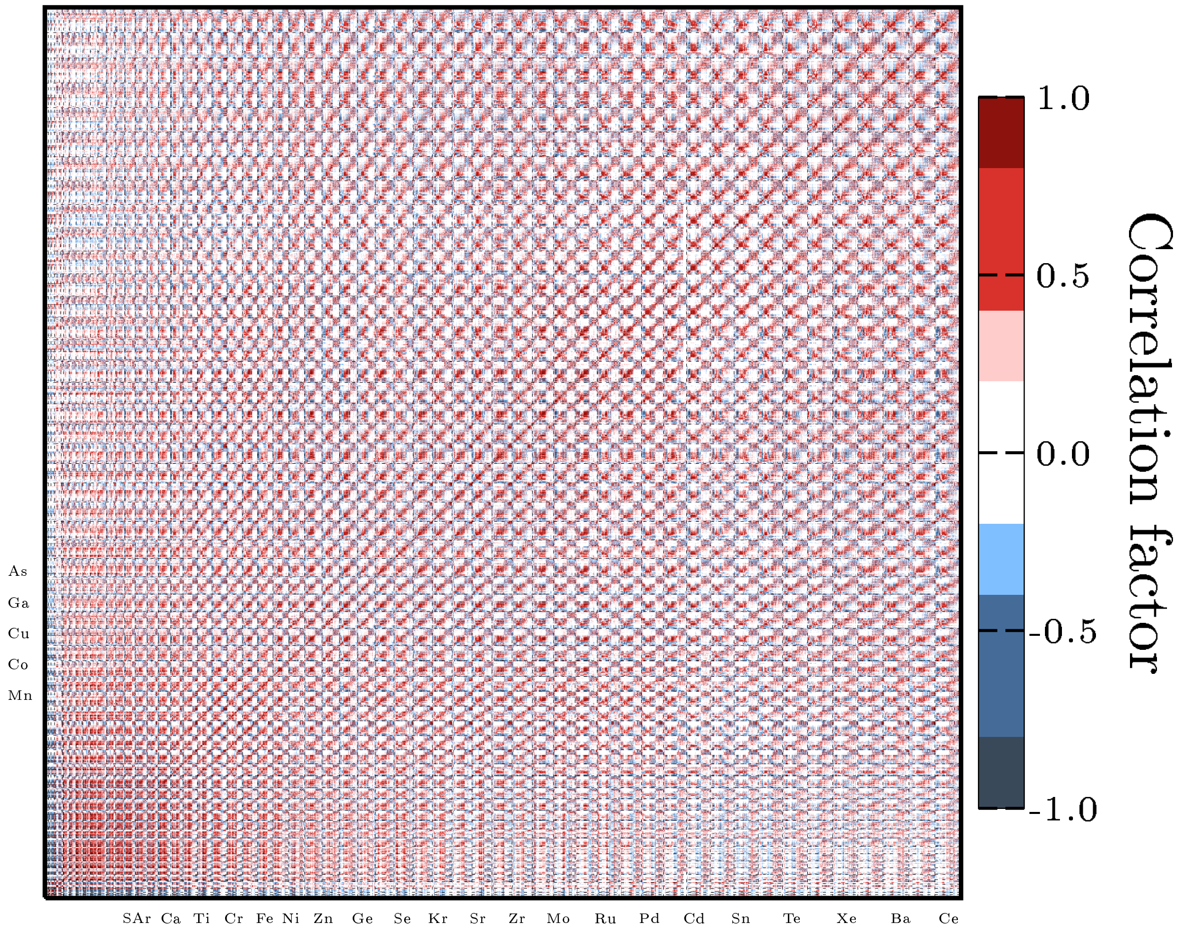



Figure 5: Correlation between nuclei for the MACS at 30 keV, taking into account 288 variations of models. Each element, included in one box, is presented with increasing mass.

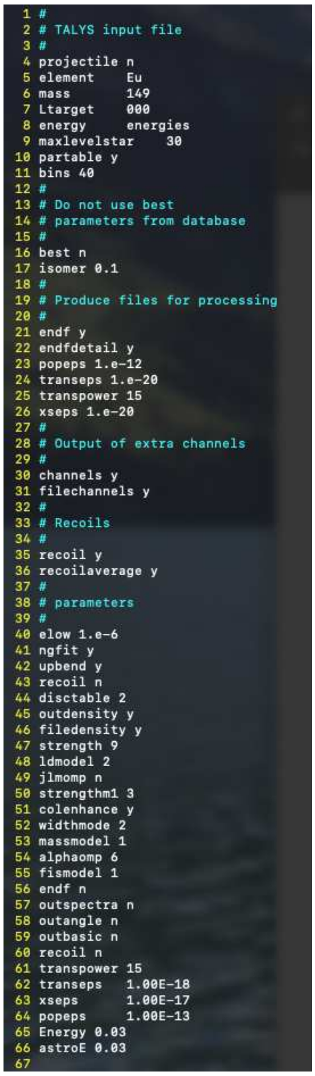
X- and Y-axis are presenting the element with increasing mass from the left to right (and from the bottom to the top). Isotopes of the same element are strongly correlated with each other (with some exceptions), but elements are also correlated with each other. It means that certain model sets provide systematically high (or low) MACS values, almost independently of the mass and charge of the isotopes. This indicates that a specific selection of models globally and systematically influences cross sections (and other quantities) for all isotopes and therefore subsequent calculations based on these cross sections.

## 4 Future developments

As mentioned, all the calculations described in the previous sections are included in the TENDL-2021 library and can be accessed online through the TENDL website (https://tendl.web.psi.ch/tendl_2021/tar_files/astro/astro.html). This is the first attempt to quantify systematically the effect of model variations. A long term goal is to update the Brussels nuclear library for astrophysics applications, called BRUSLIB [12]. Such a library contains more calculated values than the ones previously presented. It is therefore planned to update the current results with the addition of the following calculations:

- cross sections for the (n,p), (n,$\alpha$), (p,$\alpha$), (p,n), (p,$\gamma$), ($\alpha$,n), ($\alpha$,p) and ($\alpha$,$\gamma$) cross sections from TALYS,
- include model variation for fission (keyword *fismodel* in TALYS) for masses greater than 209, using either empirical fission barriers or WKB approximation for fission path model,
- include model variation for the alpha optical potential (keyword *alphaomp* in TALYS), using either the double folding model from Demetriou and Goriely, or the alpha potential of Avrigeanu (default).

In total, 9 reactions will be provided, and for each of them, either 480 model variations for atomic masses lower or equal to 209, or 960 model variations for $A > 209$. An example of a typical TALYS input for $^{149}$Eu, for the calculation of the MACS at 30 keV, is presented in Fig. 6. Similar types of input files are used for calculating all required quantities. This large number of calculations is currently ongoing and results planned to be released after 2022.



```
#
# TALYS input file
#
projectile n
element    Eu
mass       149
Ltarget    000
energy     energies
maxlevelstar    30
partable y
bins 40
#
# Do not use best
# parameters from database
#
best n
isomer 0.1
#
# Produce files for processing
#
endf y
endfdetail y
popeps 1.e-12
transeps 1.e-20
transpower 15
xseps 1.e-20
#
# Output of extra channels
#
channels y
filechannels y
#
# Recoils
#
recoil y
recoilaverage y
#
# parameters
#
elow 1.e-6
ngfit y
upbend y
recoil n
disctable 2
outdensity y
filedensity y
strength 9
ldmodel 2
jlmomp n
strengthm1 3
colenhance y
widthmode 2
massmodel 1
alphaomp 6
fismodel 1
endf n
outspectra n
outangle n
outbasic n
recoil n
transpower 15
transeps   1.00E-18
xseps      1.00E-17
popeps     1.00E-13
Energy 0.03
astroE 0.03
```

Figure 6: Typical TALYS input file for the calculation of the 30 keV MACS of $^{149}$Eu.

## 5 Conclusion

We have presented in this work the effect of modifying TALYS reaction models for the calculations of various quantities related to astrophysics. In total, 288 model sets were used, varying mass models, width fluctuation corrections, level densities, gamma-ray strength functions and optical models. Simple comparisons with covariance matrices obtained from the variation of model parameters, for a fixed model, indicated strong changes. For isotopes far from the stability line, where default models are not always adequate, uncertainties and correlations determined by varying models help to understand systematic biases of models, found to be significantly larger than the ones coming from parameter variations (for a single model). All calculated values are included in the TENDL-2021 library, and it is planned to extend this database to other reaction channels, including fission and alpha captures.

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