# FORTHCOMING APPROACHES IN NUCLEAR DATA EVALUATION

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*Received 30 April 2017; accepted 16 May 2017*

## 1. Introduction

The field of nuclear data processing belongs to fundamentally developed areas of nuclear physics and engineering as a ground state of universal knowledge. Experiments and measurements served the role of prime examination methods for centuries, developing state of art theories and explaining concealed phenomena. Despite the extensive development of nuclear data libraries in last decades [1], new methods are still being developed and point out unexpected discrepancies in values e.g. cross sections, nuclear parameters and others [2]. This paper concerns about a nuclear model computational package TALYS with emphasize on long-lived fission products – LLFP's microscopic capture cross section, as a join to previous experimental measurements on related isotope $^{128}$Te [3]. One option of reducing nuclear waste activity is via transmutation technologies. These comprise neutron capture reaction and transmutation of long living radioactive materials into less harm respectively stable isotopes.

## 2. Theoretical background

Neutron capture reaction occurs, when the target nucleus captures incident projectile in the means that compound nucleus is formed. The excitation energy of compound nucleus is at least equal to the projectile separation energy in the compound system. The theoretical interpretation is, however, somewhat disparate. In [4], the formation of compound nucleus is referred to two different mechanism: (1) - the process of the capture of the projectile in the target nucleus to form a compound nucleus with subsequent emission of a particle or gamma or (2) – the multiple emission process of highly excited residual nuclei formed after binary reaction (multiple compound emission). Besides this interpretation a pre-equilibrium reactions (*pre-compound, multi-step processes*) fill the gap between compound nucleus formation and direct reactions. These processes cover a significant part of the reaction cross section for incident energies up to hundreds MeV. Pre-equilibrium reactions give intermediate option for a memory-preserving, sometimes anisotropic, direct-like processes. Theory is widely described at [4] and [5].

The compound nucleus formation obeys angular momentum, energy and parity conservation as seen in Eq.(1).

$$\begin{gathered} E_a + S_a = E_{a'} + E_x + S_{a'} = E^{tot} \\ s + I + l = s' + I' + l' = J \\ \pi_0 \Pi_0 (-1)^l = \pi_f \Pi_f (-1)^{l'} = \Pi \end{gathered} \tag{1}$$

The binary cross section for the compound nucleus formula is given by

$$\begin{aligned} \sigma_{\alpha\alpha'}^{comp} = D^{comp} \frac{\pi}{k^2} \sum_{J=mod\,(I+s,1)}^{l_{max}+I+s} \sum_{\Pi=-1}^{1} \frac{2J+1}{(2I+1)(2s+1)} \sum_{j,l,j',l'}^{J+I,j+s,J+I',j'+s'} \\ \times\ \delta_\pi(\alpha)\delta_\pi(\alpha') \frac{T_{\alpha l j}^J(E_\alpha)\,\langle T_{\alpha' l' j'}^J(E_{\alpha'})\rangle}{\sum_{\alpha'',l'',j''} \delta_\pi(\alpha'')\,\langle T_{\alpha'' l'' j''}^J(E_{\alpha''})\rangle} W_{\alpha l j \alpha' l' j'}^J \end{aligned} \tag{2}$$

Where $E_a$- projectile energy, $s$ – projectile spin, $\pi_0$ – projectile parity, $l$ – projectile orbital angular momentum, $j$ – projectile total angular momentum, $D_{comp}$ – depletion factor for direct and pre-equilib.effects, $\alpha$ channel designation of the initial system, $T$ – transmission coefficient, $W$ – width fluctuation correction factor, $k$ – wave number of relative motion, and effective transmission coefficient for an excitation energy bin with width $\Delta E_x$ as follows

$$\langle T^J_{\alpha' l' j'}(E_{\alpha'})\rangle = \int_{E_x-\frac{1}{2}\Delta E_x}^{E_x+\frac{1}{2}\Delta E_x} dE_{x'}\rho(E_{x'}, J, \Pi) T^J_{\alpha' l' j'}(E_{\alpha'})$$

where $\rho$ is the level density [4].

ENDF/B-VII.1 library's database [1] was used as a resonance parameters source in calculation. The other options of TALYS computational system, namely JENDL-4.0 and JEFF-3.2 databases were neglected due to fact ENDF/B-VII.1 was chosen as the reference cross section library in comparison to our present results.

The output of the calculation itself does not offer a comprehensive solution, but rather partial files forming a jigsaw result. Obviously, it remains on user's intention to favor pertinent method for designated region. The TALYS code offers considerably intuitive way advising its users to determine borders easily. Thermal and Resolved Resonance Region - RRR were constructed from resonance parameters with calculation based on Multilevel Breit-Wigner MLBW formalism.

Unresolved Resonance Region – URR and fast neutron region were calculated by means of phenomenological optical model formalism. Description of this method is beyond the scope of this paper and can be found in [2] [6]. Calculation was done by subroutine ECIS-06 code system developed to solve coupled differential equations arising in nuclear model calculation by P. Moldauer [7].

## 3. Computational software

TALYS-1.8 is the latest version of TALYS code. It is copylefted free software under terms of the GNU General Public License developed by NRG Petten and associated partners [2]. The main objective of the code is simulation and analysis of nuclear reactions with incident neutrons, protons, deuterons, tritons, photons, $^3$He, alpha particles with energy range 1 keV to 200 MeV with further expansion to GeV. Code is eventually capable of use in lower energy range with interpretation of previous database or systematics. The emphasize of code development follows "first completeness, then quantity" principle. We chose this package as the forthcoming nuclear reaction prediction system among more credible codes e.g. EMPIRE (BNL), GNASH (LANL) and others.

## 4. Simulation objectives and results

As mentioned before, the accent of our work is set to LLFP, namely $^{79}$*Se*, $^{93}$*Zr*, $^{99}$*Tc*, $^{107}$*Pd*, $^{129}$*I*, $^{135}$*Cs*, $^{126}$*Sn* with addition to $^{128}$*Te*. All examined isotopes are represented by two plots on incident neutron energy range from 1e-11 to 20 MeV. Results of microscopic capture cross section obtained from TALYS-1.8 code are compared to reference ENDF/B-VII.1 database in the chart. Below each is given a C/E comparison as computed (TALYS) relative to evaluated (ENDF) value. Energy input data set for TALYS contain about 70,000 pointwise values with the highest density in RRR.

4.1. $^{79}$Se

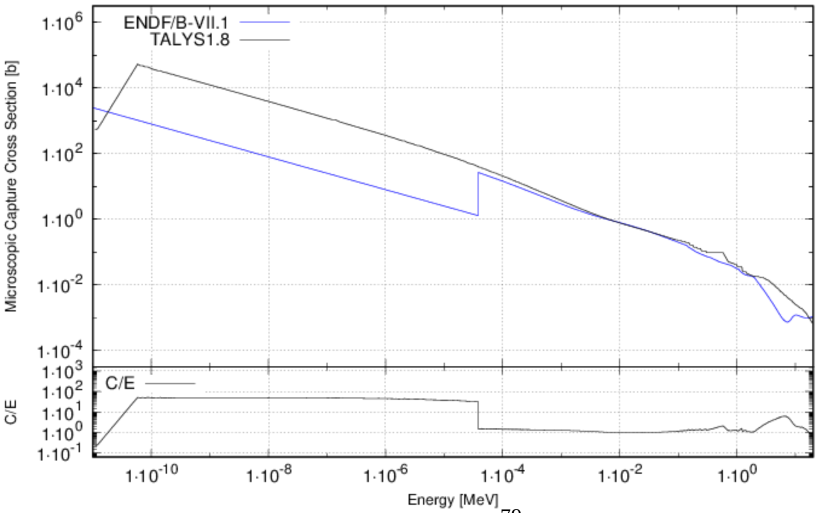


Fig.1: Comparison for $^{79}$Se isotope

4.2. $^{93}$Zr

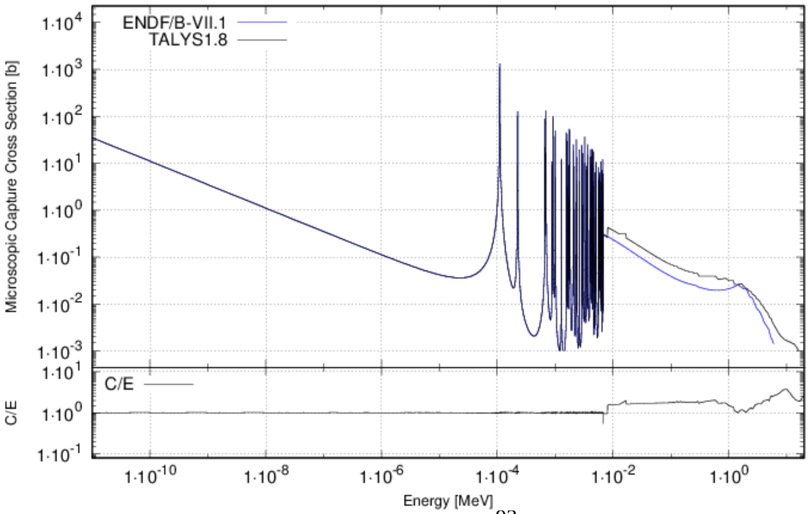


Fig.2: Comparison for $^{93}$Zr isotope

4.3. $^{99}$Tc

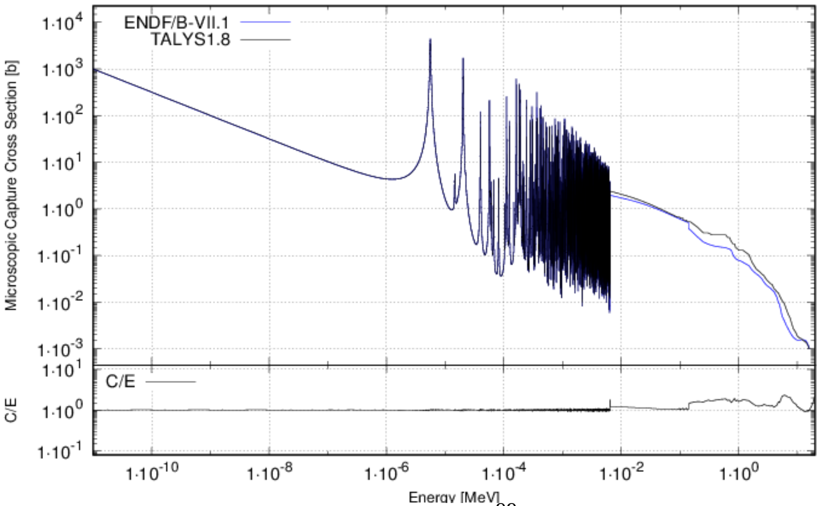


Fig.3: Comparison for $^{99}$Tc isotope

## 4.4. $^{107}$Pd

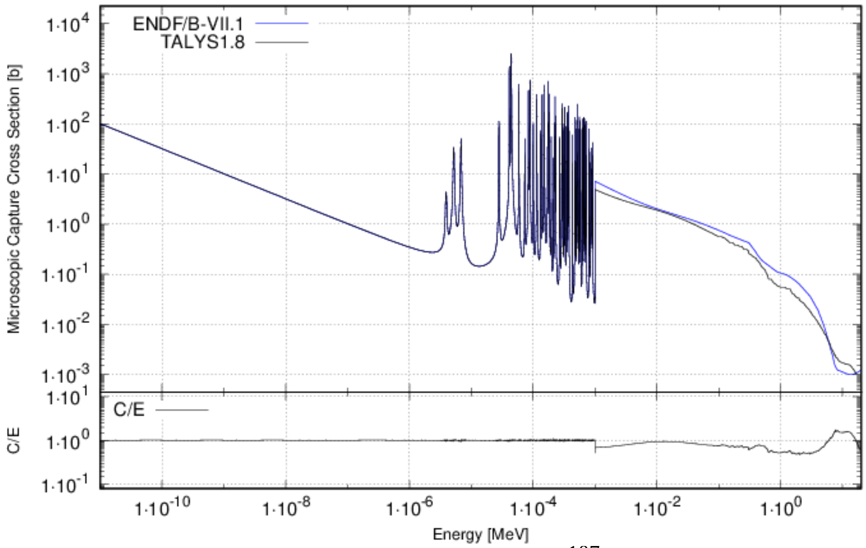


Fig.4: Comparison for $^{107}$Pd isotope

## 4.5. $^{129}$I

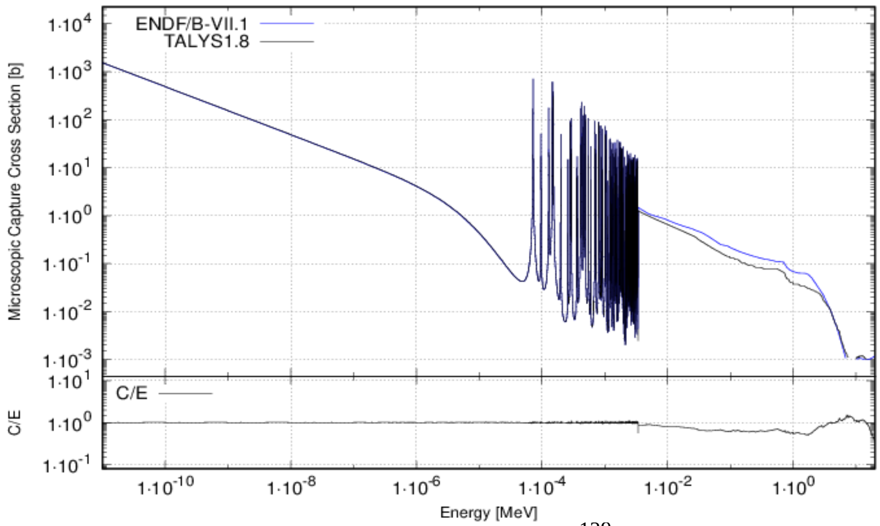


Fig.5: Comparison for $^{129}$I isotope

## 4.6. $^{135}$Cs

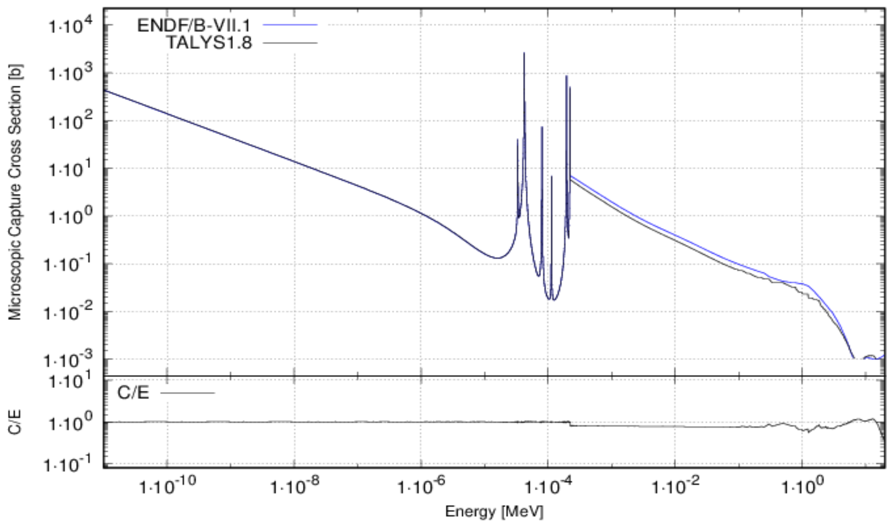


Fig.6: Comparison for $^{135}$Cs isotope

4.7. $^{126}$Sn

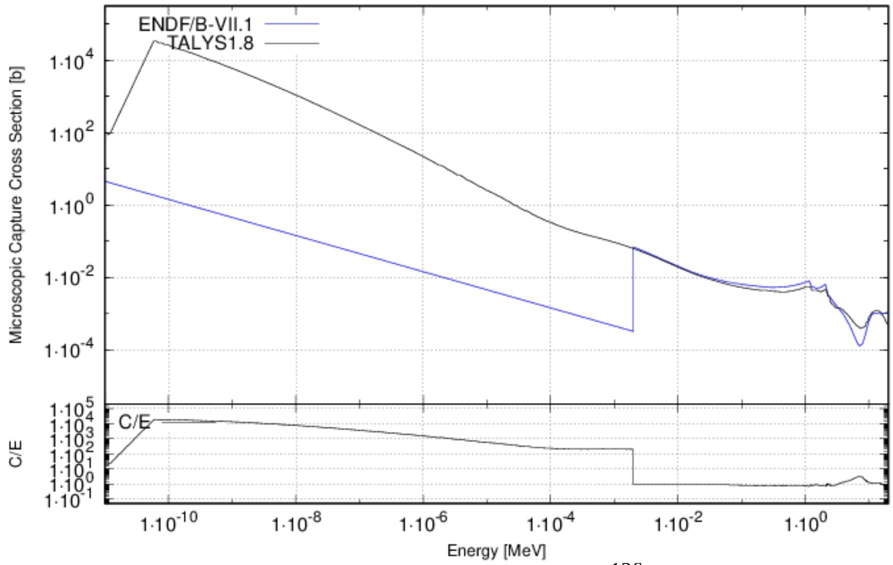


Fig.7: Comparison for $^{126}$Sn isotope

4.8. $^{128}$Te

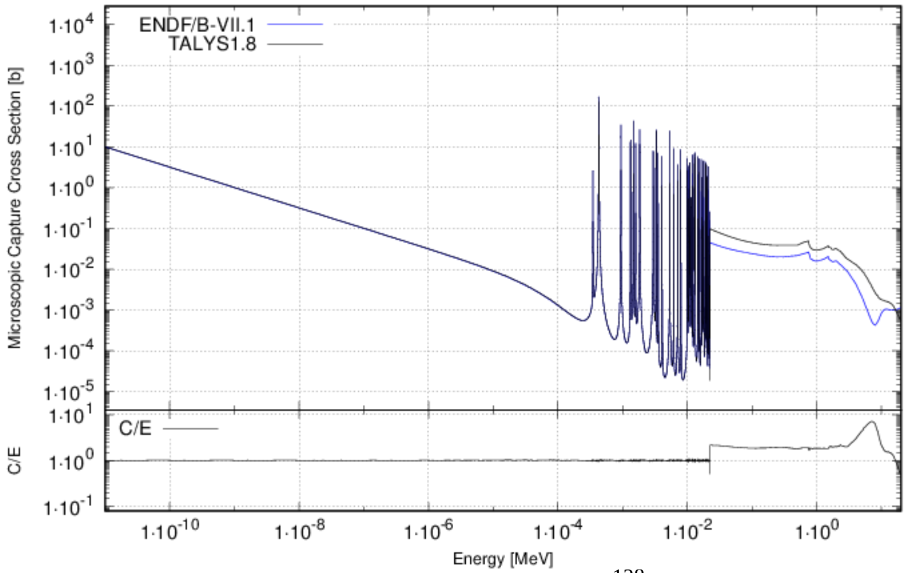


Fig.8: Comparison for $^{128}$Te isotope

## 5. Discussion

Most of the simulation results show good agreement with reference ENDF/B-VII.1 values particularly in thermal and resolved resonance region. Some discrepancy appears in fast neutron region where optical model calculations were employed. A part of the inconsistency may result from different energy bins – appearing as “steps” in characteristics (Fig. 2 and Fig. 6). However, as can be seen in some cases (Fig.1 and Fig.7), thermal region differentiates in several orders of magnitude. This may be due to fact, that $^{126}$Sn and $^{79}$Se do not possess experimental values of microscopic capture cross sections and are hence made up from evaluators’ skills and knowledge. In the end, we can state according to obtained values that TALYS code package gives values in thermal and RRR region in compliance to reference values. In fast neutron region, overestimation and underestimation appears, which might be due to chosen optical model parameters. This are in current authors' scope and their impact will be further investigated.

**Acknowledgement**
This work was financially supported by grant of Slovak Academy of Sciences No. VEGA-1/0104/17. We would like to thank Dr. Martin Petriska for technical support for simulation optimisation.

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