EMPIRE: A code for nuclear astrophysics

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Abstract. The nuclear reaction code EMPIRE is presented as a useful tool for nuclear astrophysics. EMPIRE combines a variety of the reaction models with a comprehensive library of input parameters providing a diversity of options for the user. With exclusion of the direct-semidirect capture all reaction mechanisms relevant to the nuclear astrophysics energy range of interest are implemented in the code. Comparison to experimental data show consistent agreement for all relevant channels.

1. Introduction

For the majority of elements heavier than iron, nucleosynthesis occurs mainly via neutron capture reactions in the r- and s- processes. The fission channel needs to be considered in the r-process for heavy nuclei (Z $>$ 80) [1] in which fission barriers are low. Of particular importance are the superheavy elements (SHE) since they may determine the upper end of the nucleosynthesis flow [2] which may only be reached via certain nuclear physics inputs [3]. Although the calculated and measured fission cross sections globally differ by less than a factor of three [4], current extrapolations for r-process simulation models are still unreliable. The neutron spectrum typical of s-process sites can be described by a Maxwell-Boltzmann distribution (MBD). Neutron captures have their relevant energies around the maximum of the Maxwell-Boltzmann distribution (MBD), $E_o \approx kT$ [5]. Stellar neutron capture cross sections in the mass region of the weak s-process are often not available with the required accuracy for abundance determination. The main mechanism of synthesis for the p-nuclei are photodisintegration reactions. A reprocessing of initial s-seed distribution [6] occurs via (γ,n) reactions with subsequent alpha (γ,α) or proton emission (γ,p) branchings. Simulation models have had problems reproducing the abundance distribution for the p-nuclei for Type II supernova [7]. The situation is ameliorated when considering Type 1a supernovae as a site of synthesis [8].

The heavier nuclei are formed via reactions at a high enough level density such that the Hauser Feshbach (HF) formulation applies. EMPIRE [9] is a nuclear reaction model code that accepts nucleons, γ's, and several light ions (including α-particles and deuterons) in the incoming and outgoing channels. In the presence of direct reactions, the Engelbrecht-Weidenmüller transformation can be invoked to account for the interference between compound nucleus (CN) and direct. Resonance treatment (r-matrix formalism) is beyond the scope of the code and will therefore be ignored (neutron resonances [10] can be invoked from the resonance module). The bulk of the incoming flux is treated in terms of the HF formulation with the width fluctuation correction accounted for by the HRTW [11] model. The incident channel can be treated in terms

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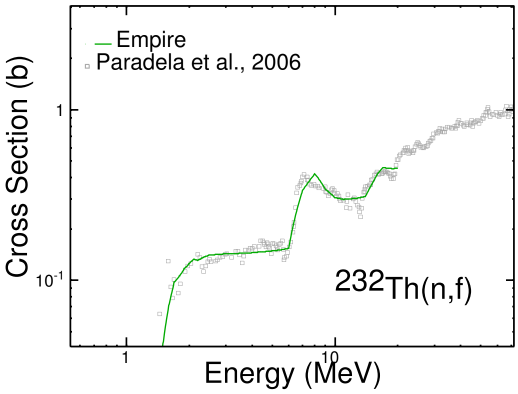

Figure 1. Neutron induced calculated cross section on ^{232}Th using EMPIRE in comparison to n_TOF [21] data

of the spherical optical model, Distorted Wave Born Approximation (DWBA), or Coupled-Channels (CC). Direct contribution to the inelastic scattering can be calculated using either DWBA or CC. The code offers an advanced fission formalism whose treatment is the optical model for fission which allows for a good reproduction of experimental fission cross sections. It offers the choice between an internal library and Hartree-Fock-Bogoliubov (HFB) fission barriers, six models for the γ-ray strength function, and level densities calculated within the Generalized Superfluid Model (EGSM), Gilbert-Cameron, or HFB combined with combinatorial method [12].

Recently, the S-factor formalism [13] [14] for non-resonant reactions (assuming a constant or very weak energy dependence within the Gamow window) has been implemented.

In the calculations below, discrete level schemes were truncated to make them consistent with the level densities. Automatic renormalization of the γ strength function was turned off in all cases [15].

2. ^{232}Th(n, f)

^{232}Th is of unique r-process origin and is a cosmochronometer (the ^{232}Th-^{238}U pair has been used to estimate the age of the r-nuclides). It has been suggested that β-delayed fission has little influence on the actinide chronometer ratios [16] but [17] suggests that spontaneous fission will affect the final abundance pattern of Th. Fig. 1 shows the fission cross section of ^{232}Th. The regional coupled-channel (CC) potential by Capote et al. [18] was used. Seven collective levels were coupled following the prescription in ref. [19]. The parabolic representation of microscopically determined HFB fission barriers were used. The barrier widths and heights were modified by less than 7% from the default values (a variation of up to 1 MeV is considered acceptable [4] [20]). In addition, the default values of the imaginary part in the optical model for the fission potential were increased. EGSM level densities were used in the main potential well and above saddles. For the gamma strength function, the Generalized Fermi Liquid Model was chosen as giving the best results. Default fission inputs were also adjusted via the number of discrete transitional states (increased from four to six), their energies, and the level densities at the saddles. One sees good agreement to the experimental data.

3. ^{186}Os(n,γ)

^{186}Os is produced via the s-process. In order to constrain the s-process contribution for ^{187}Os (Re/Os form a cosmochronometric pair) more accurate MACS are needed for the neutron capture of ^{186}Os and ^{187}Os. The modeling of ^{186}Os used the Koning-Delaroche potential [22], EGSM level densities (the level density a-parameter in the compound was scaled by 7%) and the EGLO gamma strength function (RIPL-3). The flux was treated with the spherical optical model;

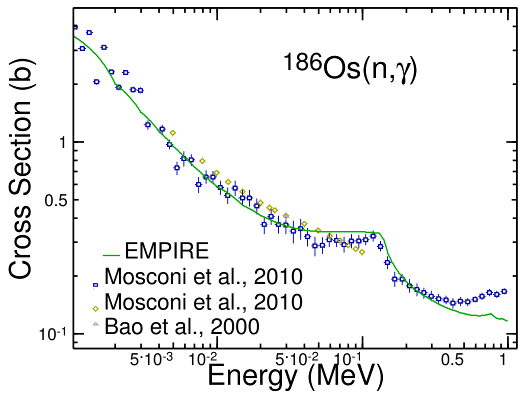

Figure 2. Neutron capture cross section of ^{186}Os using EMPIRE in comparison to the data [23] [24]

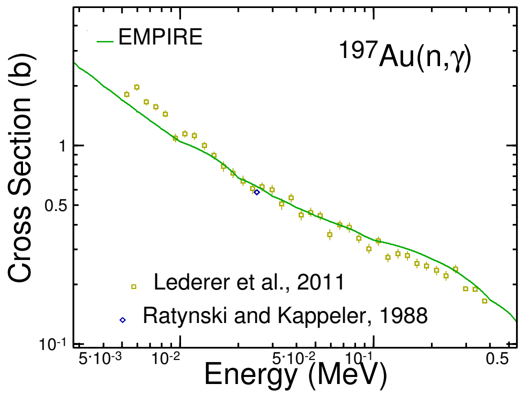

Figure 3. Neutron capture cross section of ^{197}Au using EMPIRE in comparison to the data [25] [27]

however, for those nuclei where DWBA was applied for the inelastic flux, the criterion was that the ground state deformation (β_2) should be ≤ 0.20 (^{186}Os has a β_2 of 0.20). Fig. 2 shows the calculated cross section of ^{186}Os in comparison to the experimental data. One observes a marked drop in the calculated cross section starting around 470 keV in comparison to the experimental data. Such behavior may indicate a competition cusp and/or the overestimation of the inelastic cross section (the second excited state is at 434 keV) due to the lack of a direct component.

4. ^{197}Au(n,γ)

The capture cross section of ^{197}Au [25] is well known and is used as a way to determine the neutron flux in nucleosynthesis measurements. This cross section is considered a standard from 200 keV to 2.8 MeV [26]; however, discrepancies exist with regards to the reference used for nuclear astrophysics experiments. Fig. 3 shows the calculated capture cross section of ^{197}Au in comparison to new TOF data [27]. The calculation used DWBA for the inelastic flux, the potential by Koning-Delaroche, EGSM level densities and the MLO model for the gamma strength function. Shown is the MACS from 5 to 100 keV in addition to the measured ^{197}Au cross sections (the values in the plot are energy averaged). A reasonable agreement between data and theory is observed.

5. ^{74}Se(p,γ)

Although it is photodisintegration reactions that synthesize the p-nuclei in the stellar environment, it is the inverse reaction that is generally measured in the lab. The proton branchings are more dominant at lower masses [28] and higher temperatures. The deviation between data to theory for the p-capture of p-nuclei has generally been within a factor of two (showing sensitivity between the optical potential and the level density). Fig. 4 shows the cross section and S-factor for the proton capture on ^{74}Se. This was modeled using the ESGM level densities (with a 5% adjustment via the a-parameter), the Koning-Delaroche potential, and the MLO gamma strength function. Since the ground state deformation has a value of $\beta_2 = 0.302$, CC were invoked (a default number of four levels were coupled - the conclusions of [19] don't apply for charged particles subbarrier). Although [29] states that a CC approach gives enhancements in the transmission functions for both positive and negative Q-values subbarrier, probably due to the relatively small barrier a minimal overall improvement was observed in comparison to the absense of CC (graph of spherical case not shown).

A cautionary tale should be observed when applying CC to the charged particle reactions of relevance for the γ,α and γ,p branchings in the p-process nucleosynthesis path. In principle, the effect of the coupling alters the transmission functions (the real barrier is replaced by an effective barrier) which may have implications for the nucleosynthesis when the nucleus is α-unbound (it is only the Coulomb barrier which prevents its decay). Depending on the complexity (and strength) of the feedings of a particular p-process isotope, this could potentially (artificially) alter its branch point (γ,α or γ,p). This is in contrast to DWBA where there are no coupled levels (flux is removed to uncoupled levels) and the flux is directly taken into account.

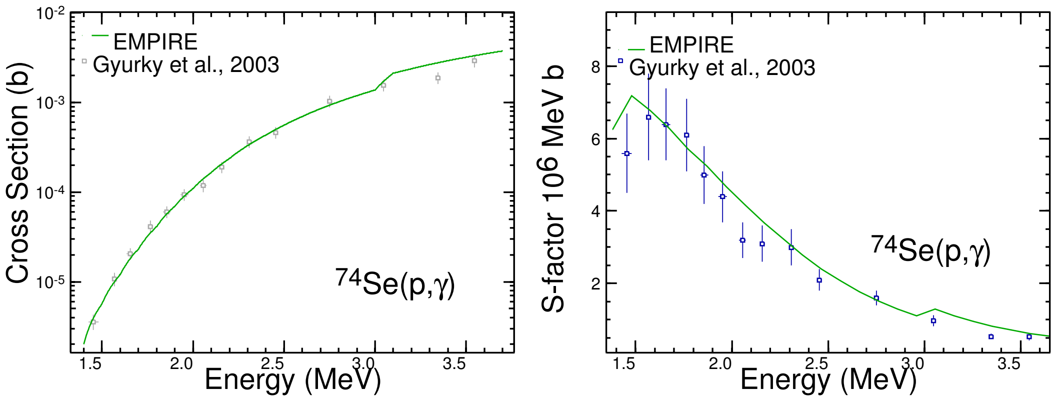

Figure 4. The cross section and S-factor for the p-capture on ^{74}Se [30]

6. ^{130}Ba+α

The agreement for α-capture has been traditionally poor mainly due to problems with the α-optical potential, although it has also been suggested that the deviations could arise due to problems with the γ width [31]. Above the neutron threshold the α-potential can be constrained by (α,n) measurements. This is in part due to the greater (α,n) cross section compared to (α,γ) and since neutron widths are generally broader any possible resonant components can often be excluded. A p-process simulation [7] within the framework of a Type II supernova showed an increased sensitivity of the abundances to a global variation of the (γ,α) and (α,γ) reaction rates in the mass region above A$\approx$ 140.

Fig. 5 shows the α-induced cross section on ^{130}Ba using both the McFadden/Satchler [33] and Avrigeanu potentials [34]. The calculation for the McFadden/Satchler potential uses DWBA for the inelastic treatment while that of the Avrigeanu potential uses the spherical optical model (no inelastic). In addition there is a 15% reduction in the volume diffuseness for the Avrigeanu

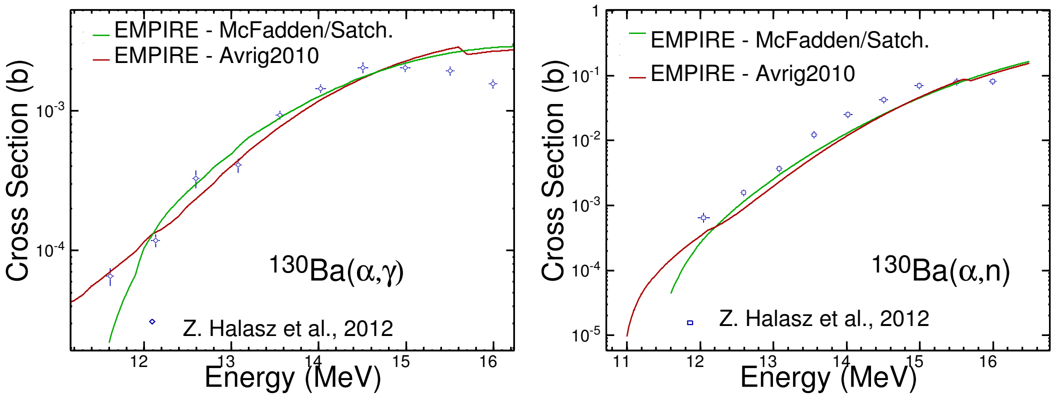

Figure 5. The cross sections for α-capture on ^{130}Ba [32]

potential. The diffuseness is considered to be one of the most sensitive parameters for the real part of the alpha potential [35]. Both use HFB level densities and the MLO model for the gamma strength function.

7. Conclusion

The calculations presented in this paper are of relevance for the r-, s- and p- processes and have been done using the reaction model code EMPIRE. The nuclear inputs are taken from the RIPL-3 database and the calculations have been performed within a nuclear astrophysics framework. The good reproduction of theory to experiment suggests it can be used as a tool for nuclear astrophysics.

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