

HNPS Advances in Nuclear Physics

Vol 30 (2024)

HNPS2023



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doi: [10.12681/hnpsanp.6200](https://doi.org/10.12681/hnpsanp.6200)

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To cite this article:

Chatziioanidis, P., & Nicolis, N. (2024). Monte-Carlo calculations of evaporation and fission in excited spallation reaction fragments. *HNPS Advances in Nuclear Physics*, 30, 233–236. <https://doi.org/10.12681/hnpsanp.6200>

Monte-Carlo calculations of evaporation and fission in excited spallation reaction fragments

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Abstract We report on a transcription of the Java program MCEF into FORTRAN. The program MCEF is suitable for fast Monte-Carlo calculations of the evaporation process and fission of highly excited fragments produced in spallation nuclear reactions. We studied the Java algorithm, analyzed the physics that govern the de-excitation process, converted the physics into FORTRAN functions, checked that the program's fundamental functions work properly, and compared the program's results to experimental data. The evaporation process translates well into the code, which has the advantage of being easily understood by the user, runs quickly, and is compatible with available related programs. Comparisons with the experimental data indicate the need for possible improvements and extensions of the present code.

Keywords Spallation reactions, Statistical model, Isotope production

INTRODUCTION

Spallation reactions are of great interest due to their usefulness in the production of radioactive nuclear beams, neutron sources, the understanding of cosmic ray abundances and the dynamics of nuclear collisions [1]. They are defined as interactions between relativistic light projectiles (usually hadrons) and heavy target nuclei. In the intermediate-energy domain, the wavelength associated with the incoming projectile is such that the interaction can be described as a sequence of nucleon-nucleon collisions referred to as the Intra-Nuclear Cascade (INC). Some of the nucleons may escape and the projectile energy is dissipated leading to a highly excited target nucleus remnant which then undergoes statistical de-excitation. This process is viewed as nucleon or cluster evaporation or γ -decay in competition with fission.

THE MCEF CODE AND ITS FORTRAN VERSION

According to Ref. [2], the MCEF code calculates emission probabilities as $P_p = G_p/G_t$ for protons, $P_\alpha = G_\alpha/G_t$ for alpha particles, $P_n = 1 - P_p - P_\alpha$ for neutrons and $P_f = G_f/(1 + G_p + G_\alpha + G_f)$ for fission. The quantities G_i are the emission widths for each de-excitation channel relative to the neutron emission width, $G_i = \Gamma_i/\Gamma_n$. They are calculated according to Weisskopf's statistical model [3] as

$$\frac{\Gamma_i}{\Gamma_j} = \left(\frac{\gamma_i}{\gamma_j}\right) \left(\frac{E_i^*}{E_j^*}\right) \left(\frac{\alpha_j}{\alpha_i}\right) \exp \left\{ 2 \left[(\alpha_i E_i^*)^{\frac{1}{2}} - (\alpha_j E_j^*)^{\frac{1}{2}} \right] \right\}. \quad (1)$$

Nuclear binding energies are calculated from the atomic masses [2,4].

Our version program (called hereafter MCEFF) reads the atomic number Z , mass number A , and excitation energy Ex of the pre-fragments from an input file and enters a do while ($Ex > 0$.AND. $A > 0$.AND. $Z > 0$) loop. In the beginning of each loop, a random number r is compared to the fission probability ($probfis$) [5]. If $r < probfis$, fission takes place, the event is recorded, and the cascade terminates. Otherwise, the emission probabilities are calculated and compared to another random number to determine which particle is emitted at each instance. At each step, the type of emitted particle

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is counted, and the remaining excitation energy of the nuclear residue is calculated. If it is negative, the cascade terminates. MCEFF outputs the total number of evaporation residues and fission events on the screen. Three output files are also created containing the mass, charge, and isotopic distributions of the final reaction products.

TESTS AND COMPARISONS WITH EXPERIMENTAL DATA

First, we tested how high excitation energies the MCEFF code may handle. Fig. 1 shows the calculated neutron, proton and alpha emission probabilities from excited ^{54}Fe and ^{58}Fe isotopes up to 1 GeV excitation energy. With increasing excitation energy, the neutron emission probability decreases whereas the proton and alpha-particle emission probabilities increase for both isotopes. Furthermore, the neutron-rich ^{58}Fe emits more neutrons and less protons and alphas than ^{54}Fe , as expected.

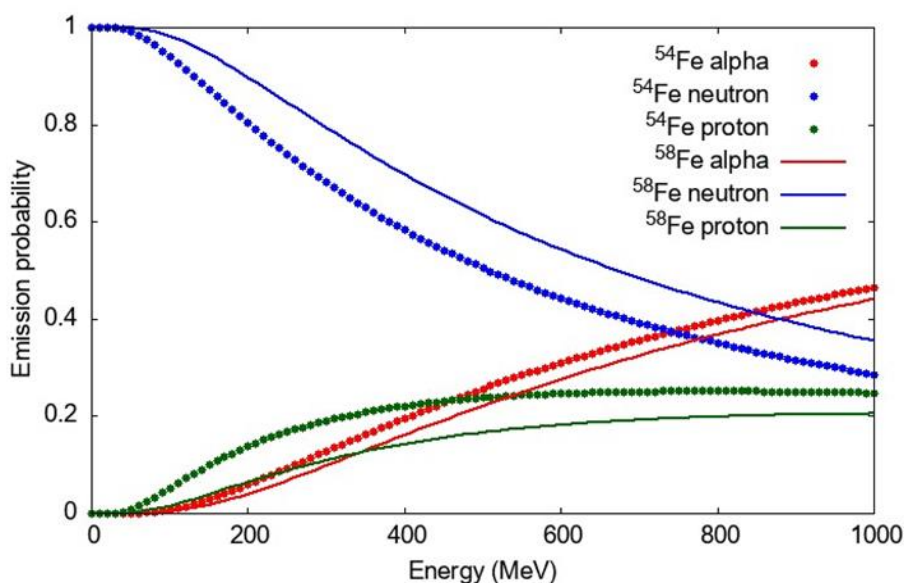


Figure 1. Calculation of the emission probabilities of alpha particles (red), neutrons (blue) and protons (green) for the ^{54}Fe (dots) and ^{58}Fe (lines) isotopes for energies up to 1 GeV

Fig. 2 shows the experimental mass distributions of the $^{56}\text{Fe}+p$ (300 MeV) reaction products from Villagrasa-Canton et al. [6] with points. The line plus open circles show the mass distribution of the excited prefragments obtained with the INC code ISABEL [7]. Following the evaporation with MCEFF, we obtain the solid line to be compared with the experimental data. The shape of the distribution above the 20mb level ($A > 45$) is reproduced whereas the region of lower masses is underestimated. This is probably happening because the calculation does not consider emission of heavy fragments with $A \geq 4$. Similar results were obtained for the corresponding charge distribution.

Symbols in Fig. 3 show the experimental isotopic distributions of the $^{56}\text{Fe}+p$ (300 MeV) reaction products from Villagrasa-Canton et al. [6]. Cross sections of isotopes with $22 \leq Z \leq 27$ are shown. The calculation with ISABEL-MCEFF is shown with the solid lines. For each Z , the calculated distributions are wider than the experimental ones and overpredict the cross section of the neutron deficient isotopes. Their magnitude is lower than the experimental and gets smaller as Z decreases. Thus, most calculated cross sections with $A \lesssim 50$ involve isotopes more neutron deficient than the data suggest.

Symbols in Fig. 4 show the experimental mass distributions of the $p + {}^{27}\text{Al}$ (180 MeV) reaction products from Kwiatkowski et al. [8]. The primary distribution is shown with the solid line plus open

circles and the final distribution after evaporation is shown with the solid line. We have an overprediction of the heaviest and an underprediction of the lowest masses.

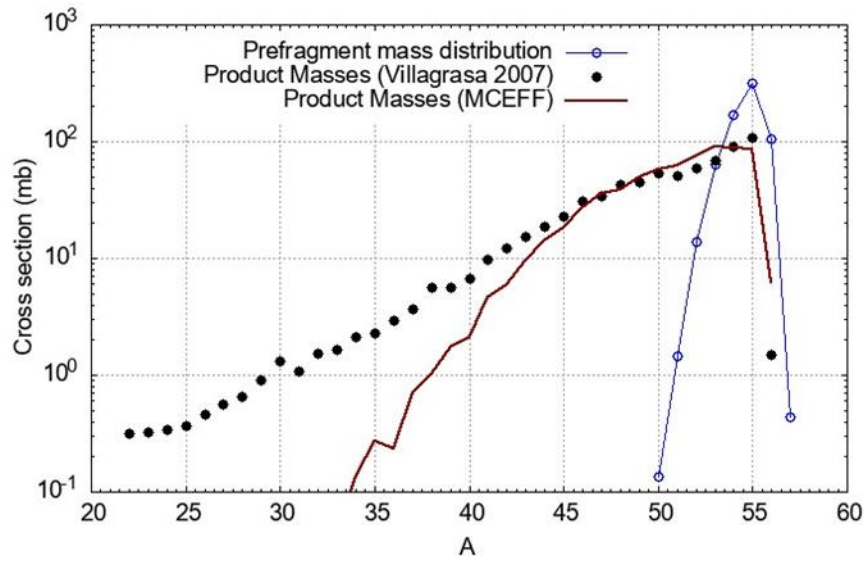


Figure 2. Mass distributions of the $^{56}\text{Fe}+p$ (300 MeV) reaction products from Villagrasa-Canton et al. [6] compared to the ISABEL-MCEFF calculations

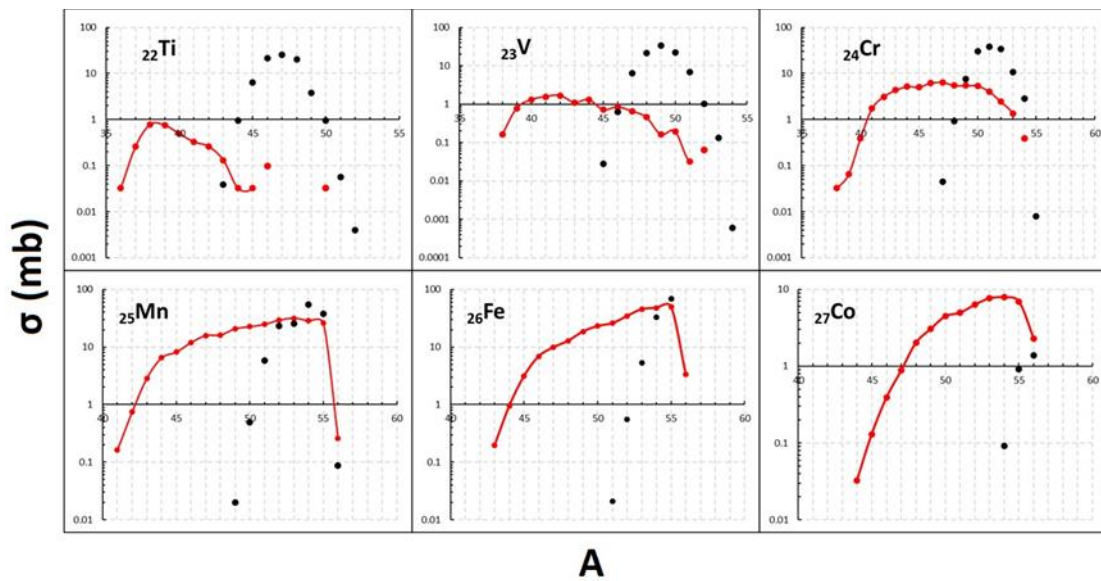


Figure 3. Isotopic distributions of the $^{56}\text{Fe}+p$ (300 MeV) reaction products from Villagrasa-Canton et al. [6] compared to the ISABEL-MCEFF calculations for $Z=22-27$

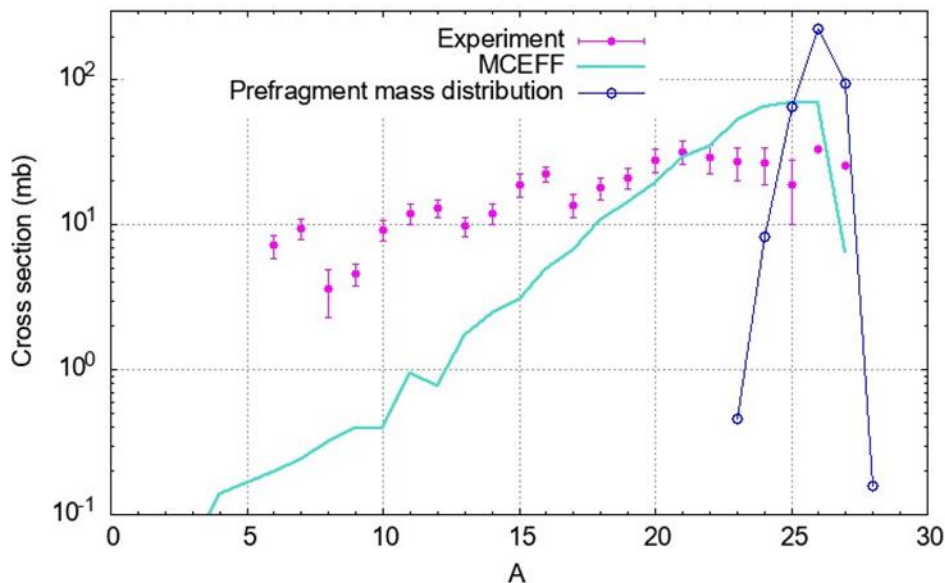


Figure 4. Mass distributions of the $p+^{27}\text{Al}$ (180 MeV) reaction products from Kwiatkowski et al. [8] compared to the ISABEL-MCEFF calculations

CONCLUSIONS

The MCEFF program is suitable for executing fast calculations of the evaporation-fission mechanism of highly excited fragments produced in spallation reactions. Tests were performed on two reactions. In both cases, the code was found to describe only the gross features of mass and charge distributions. Improvements are needed to produce more accurate predictions of the isotopic distributions. Additional work is in progress to account for the missing cross sections of low A and Z reaction products as well as their isotopic distributions. Apart from the consideration of heavy fragment evaporation, the N/Z dependence of decay modes controlled with the level density parameters and the evaporation thresholds for n, p and α emission are currently being tested.

Acknowledgments

The authors thank Professor G.A. Souliotis, Laboratory of Physical Chemistry, Department of Chemistry, University of Athens for providing the event files produced with the code ISABEL.

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