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Improvements to the evaporation code ABLA (GSI)

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1. Introduction

In a spallation reaction, it is standard to distinguish between two separate stages. The first stage is usually modelled by individual nucleon-nucleon collisions with intra-nuclear-cascade codes, which ends with the formation of a thermalised excited nuclear system. The second stage is described in the statistical model of nuclear reactions. Several evaporation codes have been developed for this purpose. However, since most of these codes have been designed for fusion reactions, there is specific need for a code adapted to the deexcitation process of spallation residues:

- The large range of excitation-energies and the large variety of nuclear species demands for a consistent treatment of level densities as a function of excitation energy and nuclear shape. The treatments of shell effects [Ign75] and collective excitations [Jun98] are particularly important.
- Due to the low angular momentum induced in spallation reactions, approximations which have been used for fusion reactions are not adapted.
- The dynamics of the fission process and the onset of thermal instabilities at the highest temperatures have to be considered. This demands for an explicit treatment of nuclear dynamics as a function of time.
- Modelling of fission requires considering a large variety of fissioning nuclei in a wide range of excitation energies. Available empirical formulations of nuclide distributions in fission of specific nuclei should be replaced by a model, which is based on more fundamental properties, like the potential energy landscape around saddle and scission.
- The application in complex transport codes demands for short computing times.

In the following, we first give a short overview of the ABLA code and the most important modifications, developed during the HINDAS project.

2. ABLA code

ABLA is a dynamical code that describes de-excitation of the compound nucleus through the evaporation of light particles and fission.

The probability that a compound nucleus with charge *Z,* neutron number *N* and excitation energy *E*, decay via channel ν is given by:

$$P_\nu(E) = \frac{\Gamma_\nu(Z,N,E)}{\sum_i \Gamma_i(Z,N,E)} \tag{1}$$

where *i* denotes all the possible decay channels (specifically: neutron emission, proton emission, alpha emission, fission). The particle evaporation is considered in the framework of the Weisskopf formalism. The particle decay widths can be written as [Wei37]:

$$\Gamma_\nu(E) = \frac{1}{2\pi\rho_c(E)} \frac{4m_\nu R^2}{\hbar^2} T^2 \rho_d(E - S_\nu - B_\nu) \tag{2}$$

where m_ν denotes the particle mass, S_ν is the particle separation energy, B_ν is the effective Coulomb barrier that takes into account the tunnelling through the barrier, *R* is the radius of the nucleus, T is the temperature of the residual nucleus after particle emission, ρ_c and ρ_d are the level densities of the compound nucleus and the daughter nucleus, respectively.

The density of excited states, ρ, is calculated with the well-known Fermi-gas formula [Hui72]:

$$\rho(E) = \frac{\sqrt{\pi}}{12} \frac{\exp(S)}{\tilde{a}^{1/4} E_{eff}^{\ 5/4}} \tag{3}$$

with the entropy S:

$$S = 2 \cdot \sqrt{\tilde{a} \cdot E_{corr}} = 2 \cdot \sqrt{\tilde{a} \cdot \left(E_{eff} + \delta\, U \cdot k\left(E_{eff}\right) + \delta\, P \cdot h\left(E_{eff}\right)\right)} \tag{4}$$

and the asymptotic level-density parameter $\tilde{a}$ as given in Ref. [IgI75]:

$$\tilde{a} = 0.073 \cdot A + 0.095 \cdot B_S \cdot A^{2/3} \tag{5}$$

where A is the mass of a nucleus, and B_s is the ratio of the surface of the deformed nucleus and a spherical nucleus. δU is the shell correction, which is for the ground state calculated as the difference between the experimental ground-state mass and the corresponding macroscopic value from the finite-range liquid-drop model [Sie86]. At the saddle point, shell corrections are assumed to be negligible. The function $k(E_{eff})$ describes the damping of the shell effects with excitation energy, and is calculated according to Ref. [Ign75] as $k(E_{eff}) = 1 - \exp(-\gamma E_{eff})$, with the parameter γ determined by $\gamma = \tilde{a} / (0.4 \cdot A^{4/3})$ [Sch82].

The effective pairing energy shift δP is calculated as:

$$\delta\, P = -\frac{1}{4} \cdot \Delta^2 \cdot g + 2 \cdot \Delta \tag{6}$$

with an average pairing gap $\Delta = 12/\sqrt{A}$, and the single-particle level density at the Fermi energy $g = 6 \cdot \tilde{a} / \pi^2$. $h(E_{eff})$ parameterises the superfluid phase transition [Ign79] at the critical energy E_{crit} = 10 MeV [Ign77]:

$$h(E_{eff}) = \begin{cases} 1 - \left(1 - \dfrac{E_{eff}}{E_{crit}}\right)^2, & E_{eff} < E_{crit} \\ 1, & E_{eff} > E_{crit} \end{cases} \tag{7}$$

The effective energy E_{eff} is shifted with respect to the excitation energy E to accommodate for the different energies of even-even, odd-mass, and odd-odd nuclei:

$E_{eff} = E$ odd – odd
$E_{eff} = E - \Delta$ odd mass
$E_{eff} = E - 2\Delta$ even – even.

As it was shown in Ref. [Jun98], collective excitations can contribute considerably to the nuclear level density. In deformed nuclei, the most important contribution to the collective enhancement of the level density originates from rotational bands, while in spherical nuclei the collective enhancement is caused by vibrational excitations.

In ABLA, the contribution of collective excitation to the level density is described in the following way: For nuclei with a quadrupole deformation $|\beta_2| > 0.15$, the rotational enhancement factor $K_{rot}(E_{corr})$ is calculated in terms of the spin-cutoff parameter $\sigma_\perp$:

$$K_{rot}(E_{corr}) = \begin{cases} \left(\sigma_\perp^2 - 1\right) \cdot f(E_{corr}) + 1, & \sigma_\perp^2 > 1 \\ 1, & \sigma_\perp^2 < 1 \end{cases}$$

$$\sigma_\perp^2 = \frac{\Im_\perp \cdot T}{\hbar^2}, \quad f(E_{corr}) = \left(1 + \exp\left(\frac{E_{corr} - E_c}{d_c}\right)\right)^{-1}$$

where E_{corr} is defined in Eq. (4), $\Im_\perp = \frac{2}{5} m_0 \cdot A \cdot R^2 \left(1 + \beta_2 / 3\right)$ is the rigid-body moment of inertia perpendicular to the symmetry axis, and m_0 is the mass unit. The ground-state quadrupole deformation β_2 is taken from the finite-range liquid-drop model including microscopic corrections [Möl95], while the saddle-point deformation is taken from the liquid-drop model as given in Ref. [Coh63]. The damping of the collective modes with increasing excitation energy is described by a Fermi function $f(E)$ with parameters E_c = 40 MeV and d_c = 10 MeV. The vibrational enhancement for spherical nuclei is generally smaller than the rotational enhancement for deformed nuclei. For nuclei with a quadrupole deformation $|\beta_2| < 0.15$, the vibrational enhancement factor is calculated as $K_{vib}(E_{corr}) = 50 \cdot \beta_{eff}^2 \cdot K_{rot}(E_{corr})$, where β_{eff} is a dynamical deformation parameter: $\beta_{eff} = 0.022 + 0.003 \cdot \Delta N + 0.005 \cdot \Delta Z$. ΔN and ΔZ are the absolute values of the number of neutrons and protons, respectively, above or below the nearest shell closure. More details about collective enhancement can be find in Ref. [Jun98].

Finally, the total level density is calculated as the product of the intrinsic level density given by Eq. (3) and $K_{vib}(E_{corr})$ and $K_{rot}(E_{corr})$.

To define the fission-decay width, apart from the level densities, the necessary ingredients are also dissipation effect that will be described in the next subsection and fission barriers. The angular-momentum dependent fission barriers are taken from the finite-range liquid-drop model predictions of Sierk [Sie86]. In order to describe the fission-fragments mass and charge distributions, as well as their kinetic energies, the ABLA code is coupled to the semi-empirical fission model PROFI. This code will be described in Section 3.

2.1. Time-dependent fission width

The modelling of the fission decay width at high excitation energies requires the treatment of the evolution of the fission degree of freedom as a diffusion process, determined by the interaction of the fission collective degree of freedom with the heat bath formed by the individual nucleons [Kra40, Gra83]. Such process can be described by the Fokker-Planck equation (FPE) [Ris89], where the variable is the time- and dissipation-dependent probability distribution $W(x, p; t, \beta)$ as a function of the deformation in fission direction x and its canonically conjugate momentum p. β is the reduced dissipation coefficient. The solution of the FPE leads to a time-dependent fission width $\Gamma_f(t)$. The results for the case of ^{238}U at a temperature of 3 MeV for different values of reduced dissipation coefficient β are shown in Figure 1 with solid lines.

However, these numerical calculations are too time consuming to be used in nuclear-reaction codes. Therefore, in most of the model calculations one of the following approximations for the time-dependent fission width $\Gamma_f(t)$ is used:

- A step function that sets in at time τ_f: $\Gamma_f(t) = \begin{cases} 0, t < \tau_f \\ \Gamma_f^k, t \geq \tau_f \end{cases}$ (8)
- An exponential in-growth function: $\Gamma_f(t) = \Gamma_f^k \{1 - \exp(-t / \tau)\}$ (9)

where $\tau = \tau_f / 2.3$, with τ_f beeing the transient time defined [Bha86] as a time in which $\Gamma_f(t)$ reaches 90% of its asymptotic value given by the Kramers fission width Γ_f^k [Kra40].

These approximations strongly deviate from the numerical solution and thus severely influence the results [Jur01]. Therefore, a new highly realistic description of the fission width based on the analytical solution of the FPE when the nuclear potential is approximated by a parabola was developed [Jur03].

The new analytical solution is based on the following assumptions: 1.) The shape of the probability distribution at the barrier deformation as a function of the velocity v is constant and only its height varies with time, 2.) For $W_n(x = x_b; t, \beta)$ the solution of the FPE obtained using a parabolic nuclear potential [Cha43] can be used, and 3.) Zero deformation and zero velocity are considered as initial conditions. In addition, the zero-point motion was taken into account by shifting the time scale by the time needed to establish the initial shape of the probability distribution. A detailed description can be found in Ref. [Jur03].

As one can see in Figure 1, this analytical approximation reproduces the exact solution for the critical damping ($\beta = 2 \cdot 10^{21}$ s^{-1}) rather well. A similar agreement is reached in the over-damped regime ($\beta > 2 \cdot 10^{21}$ s^{-1}). The approximation also gives a rather good description of the slightly under-damped motion ($\beta = 1 \cdot 10^{21}$ s^{-1}). Even in the under-damped case ($\beta = 0.5 \cdot 10^{21}$ s^{-1}), the oscillations are reproduced very well, although the absolute magnitude of the fission width is somewhat underestimated.

In the previous investigation [Jur02], it was shown that the total suppression of the fission width for small time values and the gradual increase are the most critical features of a realistic in-growth function. Both features, missing in the previously used descriptions, are well reproduced by our analytical approximation.

The actual version of the ABLA code explicitly treats the relaxation process in deformation space and the resulting time-dependent fission-decay width, using the described approximate solution of the FPE.

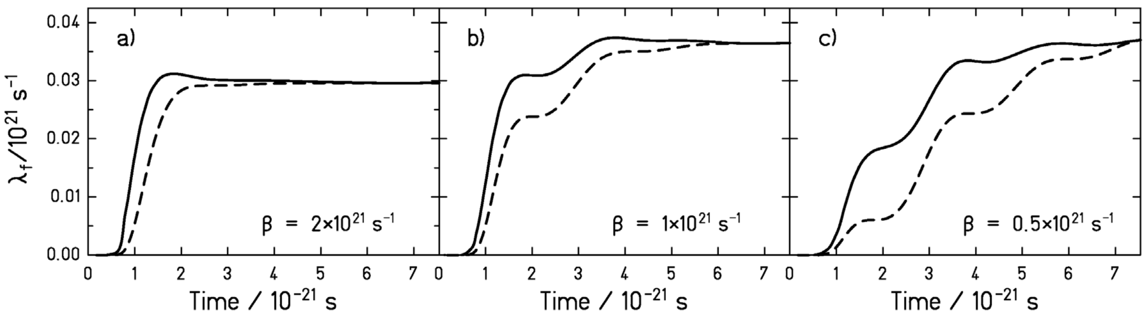

Figure 1. Fission rate $\lambda_f(t) = \Gamma_f(t) / \hbar$ as a function of time for three different values of the reduced dissipation coefficient β for ^{238}U at $T = 3$ MeV. The solid line is the numerical solution of the FPE while the dashed line is calculated using the new analytical solution as described in Ref. [Jur03].

3. The fission code PROFI

The fission code PROFI [Ben98] is a semi-empirical Monte-Carlo code developed to calculate the nuclide distributions of fission fragments. It is theoretically based on the application of the statistical model of nuclear reactions to the concept of fission channels. Within this model, the population of the fission channels is assumed to be basically determined by the number of available transition states above the potential energy surface near the fission barrier. The barrier as a function of mass asymmetry is defined by three components: The symmetric one is defined by the liquid-drop potential. Two asymmetric ones are located at mass asymmetries corresponding to neutron numbers $N = 82$ (Standard I channel) and $N \approx 90$ (Standard II channel). Three parameters (position, strength and width) of each shell are taken from channel-specific fission cross sections [Vla03] and fixed for all systems. Shells are washed out with excitation energy [Ign75]. It is assumed that the mass-asymmetry degree of freedom at the fission barrier is on the average uniquely related to the neutron numbers of the fragments. The mean values of the neutron-to-proton ratios for the channels Standard I and Standard II are deduced from measured nuclide distributions after electromagnetic induced fission of ^{238}U [Enq99]. Since the shell effects of the nascent fragments at scission, which are strongly deformed on the average, are not known experimentally, only macroscopic properties are included in the calculation of the charge polarisation of the symmetric fission channel. Consequently, the two fission fragments are obtained. Their excitation energies are calculated from the excitation and deformation energy of the fissioning system at the scission point. A full description of the model is given in [Ben98].

In Figure 2 and Figure 3 we compare the fission mass and charge distributions measured in different reactions with the prediction of PROFI code. The agreement between data and calculations is very satisfactory. The actual version of PROFI requires slight adjustments of the parameters for the different fissioning systems. It is a possible plan for the future to extend the model with one or two more parameters in order to obtain a universal version with one parameter set for all systems (up to $A_{cn} = 250$).

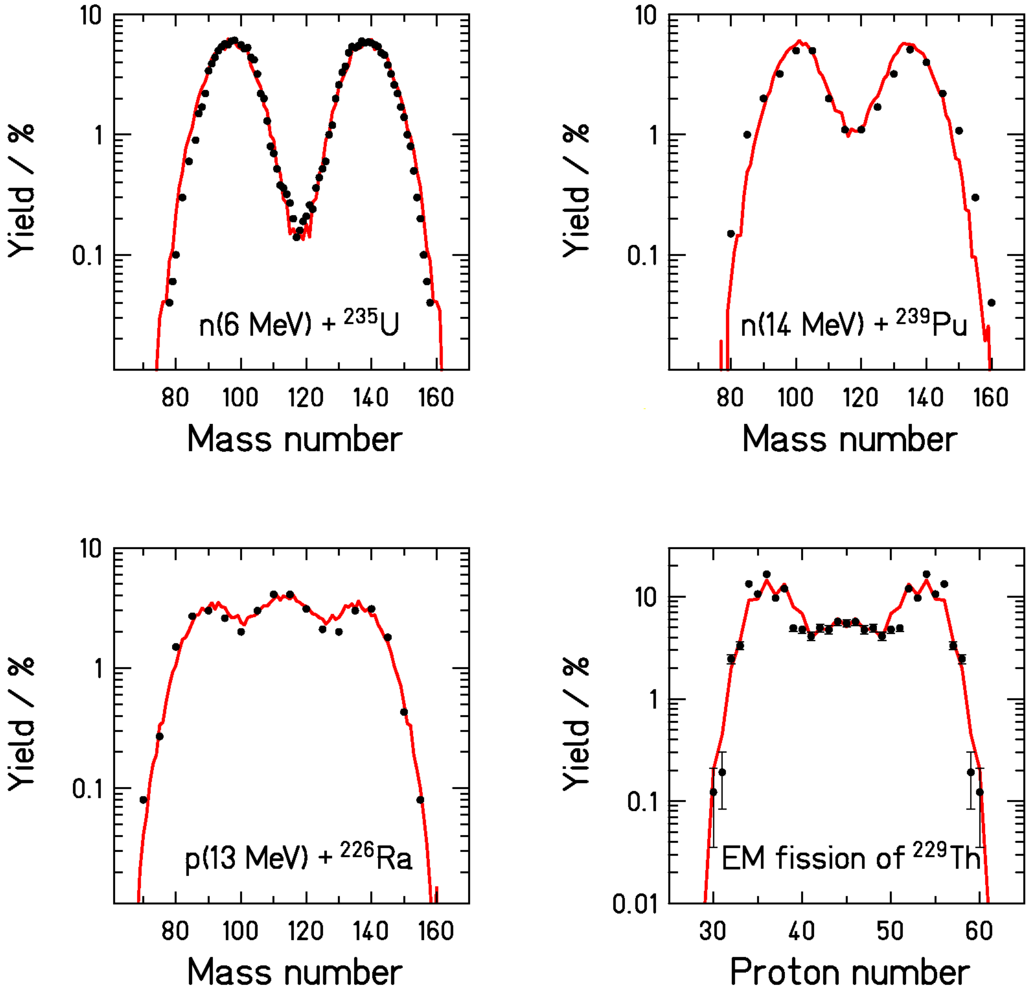

Figure 2. Comparison between experimental data (black dots) measured in the low-energy fission with the prediction of the PROFI code (red lines). Experimental data are taken from: n(6 MeV) + ^{235}U [Str87], n(14 MeV) + ^{239}Pu [Gin83], p(13 MeV) + ^{226}Ra [Per71], electro-magnetic induced fission of ^{229}Th [Sch00]. Yields are normalized to 200 %.

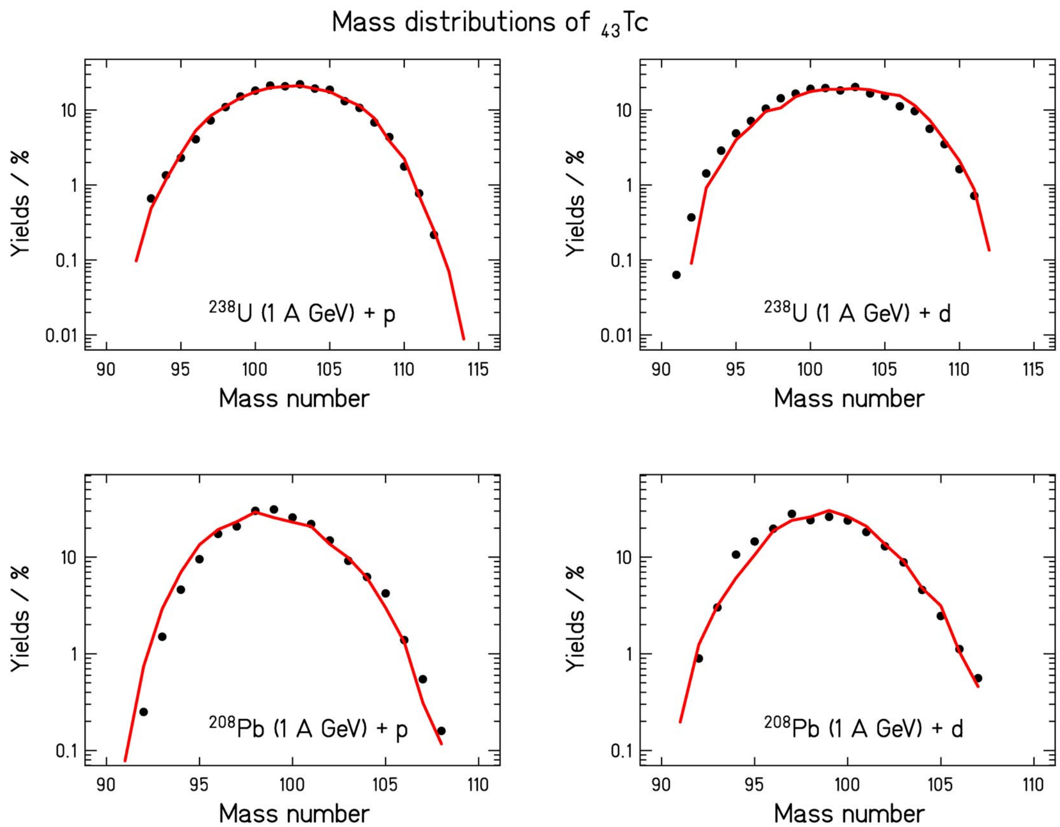

Figure 3. Mass distributions of $_{44}$Tc produced in the high-energy fission. Experimental data (black dots) measured in the frame of the HINDAS programme (see experimental contribution to the High-Energy part of the Final Report) with the prediction of our nuclear-reaction code including PROFI for the fission-fragment nuclide production (red lines). Yields are normalised to 200 %.

4. The simultaneous break-up stage

As presented in Ref. [Sch02], the analysis of the isotopic distributions of heavy projectile fragments from the reactions of a ^{238}U beam in a lead target and a titanium target gave evidence that the initial temperature of the last stage of the reaction, the evaporation cascade, is limited to a universal upper value of approximately 5 MeV. This is consistent with results on the caloric curve from multifragmentation experiments [Hau00]. The interpretation of this effect relies on the onset of the simultaneous break-up process for systems whose temperature after the first stage of the reaction (e.g. the intra-nuclear cascade) is larger than 5 MeV. In ABLA, the simultaneous break-up stage is modelled in the following way: If the temperature after the first stage of reaction exceeds the value of 5 MeV, the additional energy is used for the formation of clusters and the simultaneous emission of these clusters and several nucleons. The number of protons and neutrons emitted is assumed to conserve the N-over-Z ratio of the projectile (or target) spectator, and an amount of about 20 MeV per nucleon emitted is released. The break-up stage is assumed to be very fast, and thus the fission collective degree of freedom is not excited. The major fragment left over from the projectile (or target) spectator undergoes the sequential decay. We actually investigate a more elaborate description of the break-up process on the basis of the Statistical Multifragmentation Model (SMM) [Bon95].

In the case of spallation reactions, the break-up stage plays an important role for light targets, while for heavy targets only a small fraction of the prefragments in the upper tail of the excitation-energy distribution is formed with temperatures exceeding 5 MeV. As the consequence, the production of intermediate-mass fragments through the simultaneous break-up is more enhanced for light targets (e.g. iron). This could explain the failure of a standard evaporation model to describe the cross section for the production of intermediate-mass fragments (e.g. ^{7}Be, ^{14}C…).

4. Conclusion and outlook

During the HINDAS project important improvements in the GSI evaporation code ABLA have been performed. These improvements have profited from the high precision data measured at GSI also in the frame of the HINDAS project.

By developing the new analytical approximation to the solution of the Fokker-Planck equation for the time dependent fission width, ABLA is transformed from a pure statistical code to an dynamical code. It is coupled to the semi-empirical fission model PROFI that calculates the characteristics of fragments formed in fission. New stage, the simultaneous break-up, is introduced between the intra-nuclear cascade stage and the evaporation stage of reaction, which contributes to the production of intermediate-mass fragments.

For the future, we are planning some further development of the code, such as the inclusion of the evaporation of other light-charged particles than protons and alpha, and the emission of gamma rays. The more detailed study of the dissipation effects in fission, e.g. influence of deformation and temperature, is also planned. The fission model PROFI could be extended with one or two more parameters in order to obtain a universal version with one parameter set for all systems (up to A_{cn} = 250). Finally, we are also planning to develop more elaborate description of the break-up stage.

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