LISE++ : radioactive beam production with in-flight separators

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Abstract

The program `LISE++` is designed to predict intensity and purity for future experiments using radioactive beams with in-flight separators, as well as for tuning experiments where its results can be quickly compared to on-line data. The name `LISE++` denotes the new generation of the `LISE` program, in which any separator can be built through the use of different sections labeled "blocks". Its user-friendly interface can be used to quickly construct many separator configurations from the available blocks. The `LISE++` package already includes configuration files for most of the existing fragment and recoil separators such as the A1900 and the S800 at the NSCL, LISE3 at GANIL, FRS and SuperFRS at GSI, BigRIPS and RIPS at RIKEN, ACCULINA at Dubna. Projectile Fragmentation, Fusion-Evaporation, Fusion-Fission, Coulomb Fission, Abrasion-Fission, and two body reactions models are included in this program and can be used as the production reaction mechanism to simulate experiments at beam energies above the Coulomb barrier. This program can be downloaded free of charge from the following web sites: `http://www.nscl.msu.edu/lise` or `http://dnr080.jinr.ru/lise`.

1. Introduction

The concept of the program `LISE` [1] was elaborated during the first experiments performed on the fragment separator LISE [2] in the mid-1980s. Its aim was to simulate the operation of fragment separators used to produce radioactive beams via projectile fragmentation. One of the goals of this program is to provide a user friendly environment, designed not only to help forecast intensities and purities for planning experiments, but which can also be used as a tuning tool during experiments, where results can be quickly compared to on-line data. The choice of personal computers (PCs) to implement the program was made for two reasons:
– to make use of user-friendly features (menus, etc.);
– to ensure portability in laboratories worldwide.
However, the relatively slow speed of these systems demanded a fast algorithm to be able to perform transmission calculations in a reasonable time. The application of transport integral methods [3] to calculate the evolution of phase space distributions provides an analytical solution much faster than traditional Monte-Carlo methods.

In 1998 the program went through a number of significant changes and was ported to the "Windows" environment. LISE++ [4,5] was developed in 2001 and denotes the new generation, where users can create a separator through the use of different optical and material elements called "blocks".

The last years of the `LISE++` development were devoted mostly to the implementation of different reaction mechanisms to make `LISE++` able to simulate radioactive nuclear beams produced with in-flight fission.

We first discuss the general features of `LISE++` , with some emphasis on reaction mechanisms. We then report on new features added to the last versions, namely the expansion the Abrasion-Fission model to three regions of excitation energy, the implementation of fission reactions (Coulomb fission, Abrasion-Fission, and Fusion-Fission), the simulation of fragment production in materials, the implementation of Monte Carlo calculations for fragment transmission, the addition of an RF separator block, and the creation of a database of isomeric states.

This program is constantly evolving, guided by the feedback from users. At the time of this writing, the current version is 8.0.23, the one described in this article. Some details of the program, such as the user interface, description

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of calculation outputs and plots, and detail description of selection methods are already published in [1] and will not be repeated here.

2. General description

Projectile fragmentation and in-flight fission reactions are used worldwide in many laboratories to produce Radioactive Nuclear Beams (RNB). Being able to predict as well as identify the composition of RNBs is therefore of prime importance. These goals have shaped the main functions of LISE++:
– provide various filtering methods; the following filtering methods are available:
  · magnetic rigidity filtering ("Brho");
  · electric rigidity filtering ("Erho");
  · velocity filtering (Wien filter);
  · energy loss filtering ("Wedge" selection);
  · time selection (RF-kicker).
– simulate different RNB production reactions;
– forecast the intensity and purity of the chosen RNB;
– optimize the in-flight separator settings necessary to obtain a specific RNB;
– simulate identification plots for on-line comparison;
– provide a user-friendly graphical environment;
– enable the possibility to create different in-flight separator configurations.

2.1. Energy loss

The calculation of energy loss and energy straggling is crucial for deducing magnetic rigidities, transmission of ions and their ranges in detectors. Energy losses are calculated for atomic numbers $1 \leq Z \leq 130$ (extrapolations are available for higher Z) and energies starting at 10 keV in materials from Hydrogen to Uranium. The calculation of energy loss in gas and composite materials is also included. The following energy loss calculation methods are available:
 (i) *He*-parameterization [6]: the starting point at 2.5 AMeV is given by range tables [7].
 (ii) *H*-parameterization: TRIM code [8]
(iii) ATIMA 1.2 : LS-theory [9]
(iv) ATIMA 1.2 : without LS-corrections.

The following options are available: material inclination with respect to the beam axis, using time and energy resolutions of detectors in the calculations, detector calibration, and gas density calculator.

2.2. Ionic charge state calculations

The calculation of charge states and their corresponding transmissions can be enabled by selecting the Charge States option. When enabled, the charge states of the fragment of interest have to be specified after each dispersive block. The equilibrium charge state distribution of a beam particle after it passes through a degrading material can be calculated according to five models:

	Model	Ref.	Region
1	J.Winger	[10]	> 15 AMeV
2	A.Leon	[11]	> 5 AMeV
3	K.Shima	[12]	< 5 AMeV
4	Global	[13]	> 30 AMeV
5	G.Schiwietz	[14]	< 15 AMeV

The model used in Global allows to calculate nonequilibrium charge states distributions as well. The programs Global and Charge [13] have been incorporated into the LISE++ package and can be loaded from the LISE++ folder. These programs are intended to calculate atomic charge-changing cross sections, charge-state evolution, and equilibrium charge-state distributions of heavy ions penetrating through matter.

2.3. Optics

The optical parameters of the separator can be entered manually as standard transport matrices [15] or can alternatively be loaded from files. The emittances and energy dispersion of the primary beam are used as starting point in the transmission calculations. The program calculates the overall separator matrix using the local matrices of the optical blocks, and stores the beam vector after each of them. The envelope calculation package provides a visualization of the distributions along the separator. The evolution of horizontal and vertical angular distributions, horizontal and vertical spatial distributions, and energy and momentum distributions can be visualized.

LISE++ is restricted to first order optics at the moment, but a future adaption of the program MOTER [16] in the LISE++ package will add support for higher orders to help optimize the optics of separators.

2.4. Secondary reactions in target

The possibility to take into account multi-step reactions in thick targets has been implemented in LISE++. In this process, the projectile undergoes a series of successive reactions until the fragment of interest is produced. For the second and next reactions the program always assumes a projectile fragmentation mechanism and uses the EPAX 2.15 [17] parameterization to speed up calculations. To further expedite the evaluation of the analytical formulas of two-step reactions, and in order to include all multi-step processes, the program LISE++ uses numerical integration. For each target slice the yield of each fragment produced by secondary reactions (i.e. other than the direct one-step fragmentation) is calculated using the analytical solution based on equations of [1].

To decrease the calculation time in the case of heavy projectiles, some "acceleration filters" have been developed. The main idea of the acceleration filters is to decrease the number of intermediate parent nuclei. The filters allow the used to exclude intermediate nuclei with small contribution to the final nucleus of interest. There are two kinds of filters: "corner rectangle" (mainly for fission reactions) and "diagonal" (for projectile fragmentation) which truncate the regions where parent nuclei are calculated.

2.5. *Fragment production in degraders*

The fragment production induced by an intense secondary beams in a thick degrader (for example a wedge-shape degrader at the intermediate dispersive focal plane) can be a significant contribution to the rate of contaminants at the end of a separator. An analytical Fragment Production in Material (FPiM) model has been developed in version 8.0, which allows to qualitatively estimate this contribution. The Monte Carlo simulation was adapted to calculate the kinematics of these fragments and their transmission through the separator. Any material block can be set as a secondary target using the corresponding checkbox in the material dialog. Up to three secondary targets can be used in the program. FPiM is based on the projectile fragmentation reaction mechanism (angular and momentum distributions, `EPAX 2.15` for production cross sections). More information of FPiM can be found in [18]. Fig.1 shows a comparison between experimental data [19] obtained with the A1900 fragment separator at NSCL/MSU and the corresponding `LISE++` simulations.

2.6. *Database, mass models, mass formulas*

Accurate predictions of the production cross-sections of rare isotopes are important in the study of astro-physical processes and quest for the location of the drip-lines. Reaction models used in `LISE++` such as fission reactions or Abrasion-Ablation rely on parameterization of the nuclear masses. This may lead to large inaccuracies in case large discrepancies exist between mass parameterization and experimental masses.

The `LISE++` package contains one database based on the evaluation of atomic masses AME2003 [20], and several mass excess files which can be set as default in the calculations. The database values and their errors can be edited or plotted. The following mass excess files are included:

– *TUYY.lme* is based on the empirical mass formula with proton-neutron interaction [21];

– *HFB8.lme* and *HFB9.lme* are based on the Hartree-Fock-Bogoliubov + PLN method [22];

– *AME + Jurado2007.lme* is based on AME2003 and recent experimental data [23].

To extrapolate the masses of nuclei absent in the database the program uses an improved mass formula with shell crossing corrections developed in the `LISE++` framework [5].
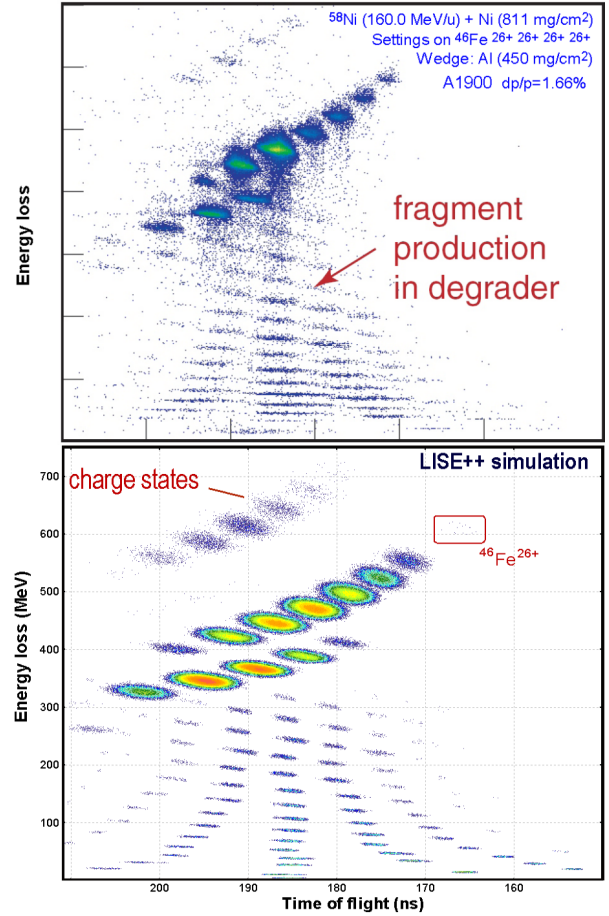

Fig. 1. Two-dimensional identification plot of energy loss versus time-of-flight. The upper panel shows the experimental data [19], while the bottom panel shows the `LISE++` simulations performed for the same settings.
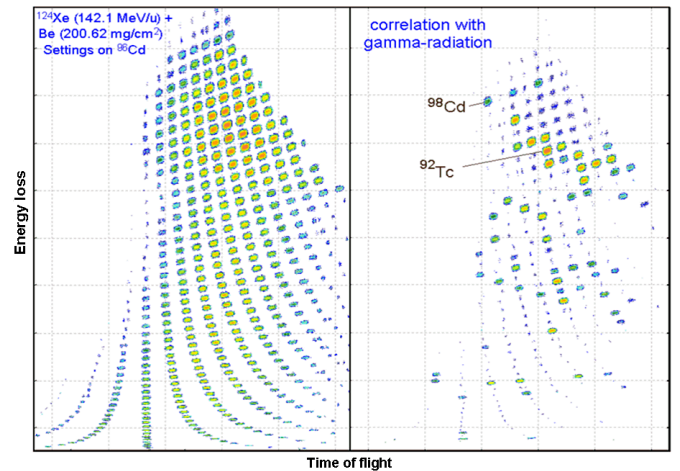

Fig. 2. `LISE++` identification plot of all nuclei produced in the reaction ^{124}Xe+Be (left panel) and those in coincidence with gamma-radiation (right panel) simulated by analogy to the work of [24] with a ^{112}Sn beam.

2.7. *Isomers in LISE++*

The fragment identification method using correlation with μs isomer states is a powerful tool in modern exper-

iments based on in-flight separation. An isomer database has been implemented in LISE++ to simulate fragment yields in coincidence with γ-ray and create an isomeric γ-spectrum and identification plot in coincidence with γ-rays (see Fig.2). The isomer database contains information (E_γ, I_{ratio}^m, $T_{1/2}$, E_{level}, I_γ, M_γ) about 2000 short-lived isomeric states extracted from NNDC, the GANIL isomer database [25] and other sources. Using this database the program is able to estimate the γ-rays yield: $Y_\gamma^m = I_{ratio}^m Y_{frag} \varepsilon_{gate} \varepsilon_{det}$, where Y_{frag} is the rate of implanted fragments, I_{ratio}^m is an isomeric transition ratio, ε_{det} is the detector efficiency, ε_{gate} is the probability to be in the γ-acquisition gate defined by $T_{1/2}$, the fragment velocity, the length of flight, and the γ-acquisition gate parameters (delay and width).

2.8. *Utilities*

Various tools developed in the LISE++ framework can be used regardless of RNB production with in-flight separators. The LISE++ package contains utilities developed within the framework of the LISE++ program as well as existing programs ported from FORTRAN to C++. The new utilities "TwinSol" and "ISOL catcher" were developed and incorporated in LISE++ in addition to the already existing tools such as the physical parameters calculator, relativistic two-body kinematics calculations, LISE library for MS Excel, evaporation calculator which allows the user to visualize the dynamics of the de-excitation process.
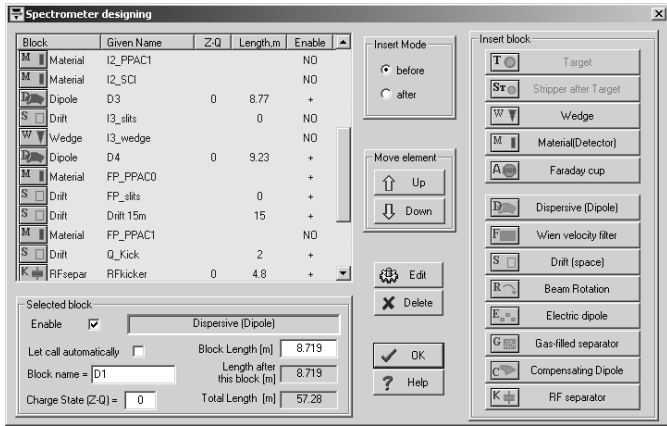

Fig. 3. The "Spectrometer design" dialog window.

3. Design your own separator

In order to overcome the limitations of the original LISE separator configuration (Dipole - Wedge - Dipole - Wien filter), allow the simulation of different in-flight separator configurations as well as the implementation of new filtering devices, LISE++ has been written in the spirit of inheritance found in object-oriented programming. For instance, the fundamental *Block* class is inherited by the *Material* and *Optical* classes. The "Spectrometer design" dialog (see

Fig.3) allows the user to construct an in-flight separator using the available blocks as seen on the figure. The spatial, angular, and energy distributions of fragments transmitted through the in-flight separator can be plotted after each block. The total and partial transmission statistics can be visualized for each block in the transmission statistic window by clicking the right button of the mouse on the isotope to be calculated in the table of nuclides.

The separator schematics is a convenient innovation (see Fig.4). LISE++ draws the separator based of the block configuration entered by the user. It is possible to select a block of the separator by clicking on it and bringing up a dialog window of its settings.

The LISE++ distribution package includes configurations for most of the existing fragment and recoil separators. Recently a new block labeled "RF kicker" has been added, which simulates a RF separator device and provides vertical beam separations for different secondary beam species due to their different time-of-flights [26].

Fig. 4. The A1900 separator navigation view in LISE++ .

3.1. *Monte Carlo calculations of fragment production and its transmission through a fragment-separator*

LISE++ (v.8.0) now allows to perform Monte Carlo calculations of fragment production in the target and/or degrader, and fragment transmission through the separator
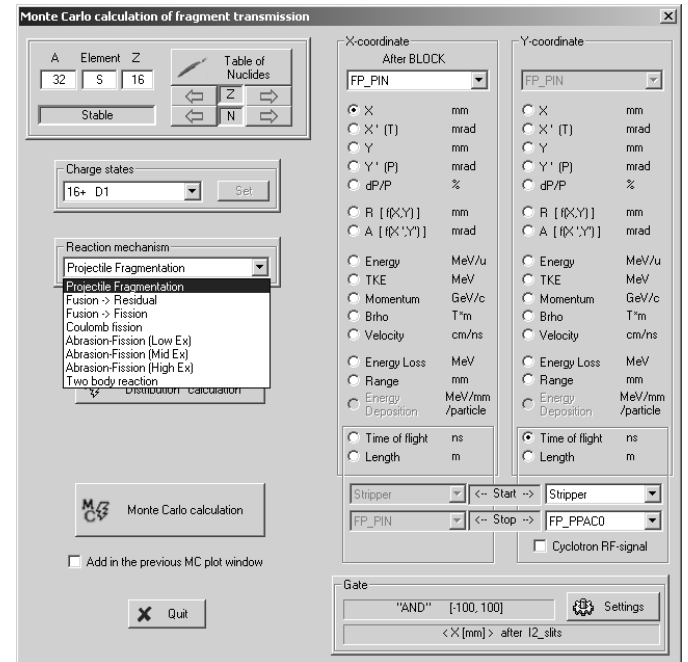

Fig. 5. The "Fragment transmission MC calculations" dialog window.

taking advantage of the block structure architecture. Before beginning the calculations the user needs to choose the two parameters to display which can be from two different blocks (see Fig.5). The Monte Carlo simulation calculates the two-dimensional plots with a frame showing the transmission value calculated at the location of the last chosen block. The "gate" option allows to apply a condition on a third independent parameter, which makes the `LISE` Monte Carlo dialog is very similar to a regular data analysis.

The Monte Carlo simulation allows to more qualitatively estimate the transmission of fragment produced in degraders. For this purpose the Monte Carlo utility uses the energy vs. position matrix created by the FPiM "Dispersion" method. The large number of available options allows the user to see the various contributions of different factors on the transmission and emittances of the secondary beams.

4. Reaction mechanisms

The development of the reaction mechanisms in `LISE++` follow these principal directions:
– Production cross-section of fragments
– Kinematics of reaction products
– Separator tuning to optimize rate (or purification)

Table 1
Reactions and production models implemented in `LISE++`

Reaction	Production cross-section model	Ref.
Projectile fragmentation	`EPAX 2.15`	[17]
	`LISE++` Abrasion-Ablation	[27]
Fusion-Residues	`LisFus` model	[27]
	`PACE4` (manually)	[28]
Fusion-Fission	`LISE++` package	[29]
Coulomb Fission	`LISE++` package	[30]
Abrasion-Fission	`LISE++ 3EER` model	[31]
Two body kinematics	`EPAX 2.15` (temporary)	

The possibility to input the cross section for a given reaction is available, provided these were actually measured or calculated by more sophisticated codes.

4.1. Evaporation cascade

Before discussing reaction mechanisms in detail it is necessary to introduce the analytical evaporation cascade [27] which was developed in the `LISE++` framework and is used in the Abrasion-Ablation model, fusion-residues and fission reactions models.

The evaporation cascade is treated in a macroscopic way on the basis of a master equation which leads to a diffusion equations as proposed by Campi and Hüfner [32], and lately reexamined by Gaimard and Schmidt [33]. The `LISE` evaporation model works with probability distributions as

a function of excitation energy, taking into account 8 possible parent and daughter channels (n, 2n, p, 2p, d, t, ^{3}He, α), as well as fission and breakup de-excitation channels. The influence of dissipation on the fission process [34] is taken into account. The analytical solution of the evaporation cascade is performed using the transport integral theory [3]. The main advantage of the `LISE` evaporation model is the speed. Only such type of fast calculations is suitable for calculating the production of nuclei with very low cross sections.

4.1.1. Fission barrier

Fission barriers are necessary to calculate fission de-excitation channels and estimate the total cross-sections of fission reactions, evaporation residue cross-sections, and decay widths in the post-scission nucleon emission process. The Cohen rotating liquid drop fission barrier model [35] was used initially in `LISE++`. A large fission yield close to the proton closed shell Z=82 it was found that the fission model doesn't agree with experimental data, which can be explained by a fission barrier too small, whereas it is expected to grow near shell closures. It was therefore necessary to introduce shell corrections and odd-even effects. The fission barrier used in the program is the sum of the calculated value in the selected model at $L = 0$, with shell and odd-even corrections: $B_f^{final} = B_f^{init} \cdot b + \varepsilon_{shell} + \varepsilon_{odd-even}$, where b (Barfac) is a multiplication factor, with a default value of b=1. This factor can be modified by the user in the Fission barrier dialog window. For shell corrections the program uses results from the `LISE++` LDM2 model [5].

The user can choose from five available options: three models (Cohen [35], Sierk [36], Myers [37]) to calculate the fission barrier, and two files: calculated fission barriers by the ET-FSI method [38], or experimental data [39]. See [31] for more details.

4.2. Projectile fragmentation

Projectile fragmentation can be pictured for example as an abrasion model followed by sequential evaporation by both projectile and target spectators fragments.

In the early versions the statistical model [40] was used by default to determine the momentum and angular phase space distributions of the projectile fragments. The fragment velocity may be set to a constant value or can be calculated from five different available methods. The shapes of the fragment momentum distributions measured in relativistic heavy ion collisions are typically Gaussian. Four models of momentum distributions and two corrections to their widths are available. Which model is relevant depends on the energy and mass of the projectile. By default the program uses `LISE`'s Universal parametrization [41].

4.3. Fusion Residues

The fusion-evaporation model `LisFus` [27] for fast analytical calculations of fusion residues cross sections is available. This model is based on the Bass fusion cross-section algorithm [42], as well as the `LISE` evaporation model discussed above (see section 4.1). The user has also the possibility to use fusion residue cross sections calculated by the program `PACE` [28], which is incorporated in the `LISE` package. In the `LISE` framework the program `PACE4` has several new features:

– User-friendly interface. A convenient output of the results is available as well as the possibility to visualize the calculated cross-sections using the `LISE` tools;

– Possibility to calculate a fusion cross section below the Coulomb barrier in `PACE4` and the `LisFus` model using the quantum-mechanical approach of C.Wong [43].

– The AME2003 database of recommended values [20] for binding energies can be used in the calculations.

4.4. Fission reactions

Secondary-beam facilities such as GSI, RIBF, NSCL, and GANIL can provide heavy beams such as ^{238}U which enable the use of fission reactions, for which fast qualitative predictions of fission fragment intensities are needed. A model of fast analytical calculation of fission fragment transmission through an in-flight separator has been developed in the `LISE++` framework. A key aspect of in-flight fission experiments is the contribution of secondary reactions in the target to the production of exotic nuclei. The program predicts that the primary fission distributions are modified greatly by secondary interactions in thick targets. These secondary interactions may provide a method to produce more exotic nuclei, in particular on the neutron-rich side.

In the following sections the details of fission modes and the kinematic models will be discussed briefly. For more details see the `LISE++` documentation [29–31].

4.4.1. Fission fragment production model

The fission fragment production model (`FisFPM`) is at the basis of all fission reactions implemented in `LISE++`. The fissile nucleus (A,Z), fission channel cross section (σ_{fis}), and excitation energy (E^*) are the input parameters of this model. In addition, the kinetic energy of the fissile nucleus is used for kinematics calculations in order to estimate the transmission through the separator.

As a first step, `LISE++` calculates an initial fission cross-section matrix of excited fragments using the semi-empirical model of J. Benlliure [44]. This model has some similarities with previously published approaches [45,46], with the added advantage of describing fission properties of a large number of fissile nuclei over a wide range of excitation energies. The macroscopic part of the potential energy at the fission barrier as a function of the mass-asymmetry

degree of freedom is taken from experiment [46]. The model also takes into account unbound nuclei as well in this stage of the calculations.

The post-scission nucleon emission is the final step of the calculation. Thanks to the `LISE` evaporation cascade model (see section 4.1) to calculate the number of post-scission nucleons, shell effects in the TKE distributions can be observed, which enables the user to make a **rapid** and **qualitative** estimate of the final fission fragment yield. Both stages of the calculation take a little less than 5 seconds in the case of low-energy fission.

Two methods for calculating fission fragment kinematics are available in `LISE++` :

– The MC (Monte Carlo) method is available for a qualitative analysis of fission fragment kinematics and can be used in the Kinematics calculator;

– The Distribution Method is the fast analytical method used to calculate the fragment transmission through all the optical blocks of the separator.

4.4.2. Coulomb Fission, Abrasion-Fission

The fission of ^{238}U can be induced by both electromagnetic and nuclear processes. At large impact parameters and for high-Z targets, the long-range Coulomb force prevails (Coulomb fission). The projectile is excited mostly to the giant resonance region by an exchange of virtual photons; it then decays by neutron emission or fission. For smaller impact parameters, peripheral nuclear collisions take place and the fissile projectile is left abraded and excited (Abrasion-Fission). After de-excitation by nucleon emission, it can undergo fission with a finite probability [47].

The electromagnetic excitation cross-section calculation is based on work of C.Bertulani and G.Baur [48]. `LISE++` calculates the statistical parameters (mean value $\overline{E}^*$, area σ_{fis}) of the de-excitation fission function ($d\sigma_{fis}/dE^*$), which are then used in the `FisFPM` model (see Section 4.4.1).

In the case of Abrasion-Fission an added complexity arises from the fact that there are more than 1000 possible fissile nuclei after abrasion of a fast heavy projectile, compared to only one fissile nucleus in the case of Coulomb fission. To overcome this problem, the LISE program models the Abrasion-Fission fragment production using three excitation energy regions (`3EER`) [31]. The model choses only three fissile nuclei for the different excitation energy regions, which are calculated using the `LISE++` Abrasion-Ablation model. The excitation regions (*low*, *middle*, *high*) are determined by three parameters: excitation energy, cross-section, and fissile nucleus (A,Z), which are entered into the `FisFPM` model.

4.4.3. Fusion-Fission

Fusion-fission reactions with heavy targets in normal kinematics are usually challenging due to difficulties with fragment extraction from the target and identification.
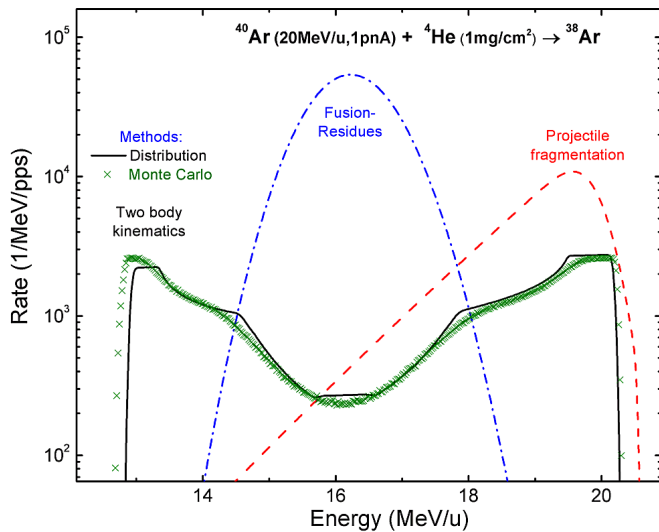
Fig. 6. Energy spectra calculated by the "Distribution" method of ^{38}Ar fragments produced by different reaction mechanisms, using an ^{40}Ar beam at 20 MeV/u on a ^{4}He target (1 mg/cm^2) and gated by a rectangular angular acceptance $X' = \pm 100 mrad$, $Y' = \pm 60 mrad$. The Monte Carlo calculation of the energy spectrum of ^{38}Ar fragment produced in two body reaction is also shown. The default `LISE++` production cross sections `EPAX 2.15` and `LisFus` model were used to estimate the rates.

With a ^{238}U primary beam however, it is possible to use an in-flight separation technique. This new production mechanism of RNB has been developed in the `LISE++` framework. Simulations show the possibility to produce new neutron-rich isotopes with Z=60-70. See [29] for more details.

4.5. Two body reactions

The Two Body kinematics calculation has been implemented using the kinematic code developed for fission reactions for the analytical method ("Distribution") transmission calculation, as well as the new `LISE` Monte Carlo (v.7.9) method (see Fig.6). The following assumptions are used:

– the distribution of fragments is isotropic in the center mass system;
– the fragments are produced in their ground state;
– the cross sections are taken from `EPAX` by default, but it is highly recommended to input realistic cross sections manually.

5. Summary

Constant improvements of `LISE++` based on suggestions by the user community has rendered this program highly versatile and flexible. It is well suited to simulate in-flight separators used in almost any nuclear physics experiment where RNBs are produced and filtered by magnetic and/or electrostatic separation devices.

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