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Possible Improvements to MCNP6
and its CEM/LAQGSM Event-Generators

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Abstract

This report is intended to the MCNP6 developers and sponsors of MCNP6. It presents a set of suggested possible future improvements to MCNP6 and to its CEM03.03 and LAQGSM03.03 event-generators. A few suggested modifications of MCNP6 are quite simple, aimed at avoiding possible problems with running MCNP6 on various computers, i.e., these changes are not expected to change or improve any results, but should make the use of MCNP6 easier; such changes are expected to require limited man-power resources. On the other hand, several other suggested improvements require a serious further development of nuclear reaction models, are expected to improve significantly the predictive power of MCNP6 for a number of nuclear reactions; but, such developments require several years of work by real experts on nuclear reactions.

1

Contents

1. Introduction

Implementation [1, 2] of the Cascade-Exciton Model (CEM) and the Los Alamos version of the Quark-Gluon String Model (LAQGSM) codes in MCNPX [3] and subsequently their further use and improvement in MCNP6 [4] extended significantly the capabilities of both these transport codes, allowing us to simulate photonuclear reactions at energies up to ~ 10 GeV, as well as reactions induced by arbitrary heavy nuclei and by almost all types of elementary particles at energies up to ~ 1 TeV/nucleon. The latest version of MCNP6, MCNP6.1.1 [5] uses the latest versions of CEM, CEM03.03 [6, 8] and LAQGSM, LAQGSM03.03 [8, 9] and became one of the most powerful Monte Carlo transport codes available today in the world.

MCNP6, using its CEM03.03 and LAQGSM03.03 event-generators, was validated and verified (V&V) on many intermediate and high-energy (i.e., above ~ 14 MeV, and up to 0.8 TeV) test-problems on both thin and thick targets bombarded with beams of particles and heavy nuclei and proved to describe the whole variety of reactions tested quite well (see, e.g., [10] – [13]). However, there are still a number of possible and desirable improvements to MCNP6 and its physics models, in order to make it a more universal transport code and to increase its predictive power for a number of reactions. Here, we discuss several such possible improvements to MCNP6 and its physics models, starting from the simplest and relatively easy to do and moving to more serious developments of nuclear reaction models, requiring a larger amount of time and man-power by real experts in high-energy nuclear reactions.

2. "Data Files" from Models

The simplest modification to MCNP6 we like to suggest concerns only about the arrangement and structure of files in the MCNP6 package and does not address at all any changes of the physics models.

MCNP6 can use at present five event-generators, namely:

1) Bertini IntraNuclear Cascade (INC) [14], followed (by default) by the Multistage Preequilibrium Model (MPM) [15] to describe emission of particles from the excited nucleus produced after INC, followed by the Dresner evaporation model [16] to describe evaporation of particles from the excited nucleus produced after the preequilibrium stage of reaction, followed by or in competition with fission, described either with the RAL [17] or with the ORNL [18] fission models, followed (if the residual nucleus has a mass number $A < 13$) by the Fermi Break-up model [19];

2) ISABEL INC [20], followed after the INC stage of reactions by the same models as in the above case;

3) Cascade-Exciton Model (CEM) code CEM03.03 [6] with its own INC, preequilibrium, evaporation, fission, and Fermi break-up models;

4) Los Alamos version of the Quark-Gluon String Model (LAQGSM) code LAQGSM03.03 [9] with its own INC, preequilibrium, evaporation, fission, and Fermi break-up models;

5) IntraNuclear Cascade developed at Liege (INCL) [21] merged with the ABLA evaporation/fission code [22].

All these models use a variety of nuclear data, like approximations for cross sections of nucleon-nucleon and other particle interactions, masses of nuclei, binding energies, fission barriers, etc. Initially, the numerical data used by each of these models were part of their FORTRAN77 codes, represented either in separate, dedicated subroutines, or as parts of other

subroutines/functions, made available through the code where needed via common blocks, and often using equivalence. With the development of more modern versions of FORTRAN, to make MCNP6 compatible with modern compilers, the old FORTRAN77 or even FORTRAN66 versions of the original physics model codes were edited and the numerous tabulated data from them were extracted in separate files or even in separate modules. By doing so, it was somehow forgotten that those tables are actually part of physics model codes; they were called "Data Files" and were rearranged in MCNP6 together with other Data Files, like the ACE files with real "Data Libraries." Because of some official regulation on using Data Libraries, the last ones are provided now in the MCNP6 package on a separate DVD. This may cause some problems of using the numerical data needed for the physical model codes, that are not related in any way with the real data libraries. Such problems actually did occur in the past, even at our MCNP6 Classes, when I was not able to run MCNP6 on a test-problem for students using the Bertini INC, because MCNP6 could not find some "Data Files" needed for the Bertini INC.

To avoid similar problems for MCNP6 users, taking into account that the regulations concerning the distribution of Data Libraries to users may change in the future, I suggest to reorganize the files of MCNP6 and place the corresponding "data files" used by the different physics models together with the corresponding FORTRAN modules of those models. This way, the users on MCNP6 would not depend on the circumstances if they have or not access to some Data Libraries, and should be able to run MCNP6 using physics models even without any Data Libraries. This modification should not change any results by MCNP6, but would prevent possible future problems of running MCNP6 with some models.

3. Low-Energy d-, t-, ^{3}He-, ^{4}He-, and Heavy-Ion-Induced Reactions in MCNP6

By default, MCNP6 uses data libraries, when available, and only at energies above the one covered by ACE data libraries (usually, 150 MeV), or for some exotic target-nuclei not covered by data libraries, uses nuclear reaction models listed in the previous section. As of today, MCNP6 uses by default data libraries only for nuclear reactions induced by neutrons, protons, and photons. Reactions induced by d, t, ^{3}He and ^{4}He on very light targets are also covered by special data libraries. But reactions induced by these complex particles (or as we refer them in MCNP6/X, "light ions") on medium and heavy target-nuclei are simulated with ISABEL, at energies below 800 MeV, and with LAQGSM at higher energies. All types of reactions induced by nuclei heavier than ^{4}He (called in the MCNP language as "heavy-ions") are simulated with LAQGSM, at all energies, even very low. This is not a good situation, as it is well known that no INC-type models, including ISABEL and LAQGSM, are expected to provide reliable results at low incident energies, below ~ 100 MeV or even much lower.

One relatively easy way to address these problems in the case of reactions induced by complex particles up to ^{4}He would be to use data libraries for such reactions. Fortunately, there are already data libraries for such reactions. So, the TENDL-2014 data library [23, 24] provides files in both ENDF and ACE formats for reactions induced by d, t, ^{3}He, and ^{4}He (as well as by n, p, and γ) on practically all stable and long-lived nuclei at energies up to 200 MeV (produced with the TALYS code).

Implementation in MCNP6 of an additional event-generator able to describe reliably low-energy heavy-ion induced reactions is suggested.

4. Extending the GENXS option in MCNP6

The GENXS option [25] of MCNP6 is a very useful capability as it allows us to tally and output in the absolute value double differential, angle- and energy-integrated spectra, and total cross sections for the production of up to 24 types of possible secondary particles produced in nuclear reactions, as well yields of all nuclei from such reactions. In a way, GENXS is a unique capability of MCNP6 allowing us to test its event-generators on interactions with a single nucleus (as we would study very thin targets), using MCNP6 input files for real thick targets, from real applications. See Ref. [25] for a full explanation of GENXS. However, as initially proposed and developed by Dick Prael, the GENXS option [25] allows us to tally spectra and yields of secondary particles (ejectiles) only up to ^{4}He: We can not use GENXS in the current official version of MCNP6 to get spectra of heavier fragments, like ^{7}Be, or of residual nuclei.

This inconvenience was recently solved by us in an internal, working version of MCNP6 (see details in Refs. [26, 27]). The GENXS upgrade includes the ability to tally and output double differential cross sections for any heavy nuclei (with valid ZAID). It also includes the ability to tally and output angle-integrated cross sections per emitted fragment energy and energy-integrated cross sections per emitted angle, for any ZAID.

As an example, Fig. 1 shows the spectrum of ^{6}Li at 20 degrees from 200 MeV p + ^{27}Al calculated by CEM03.03 and by MCNP6 with the extended GENXS. We see that the extended option of GENXS in MCNP6 provides spectra for products heavier than ^{4}He in good agreement with results obtained by CEM03.03 used as a stand-alone code. The extended version of GENXS was tested successfully also for other MCNP6 event-generators (INCL+ABLA, Bertini+Deresner+RAL, and LAQGSM03.03), as well as on reactions induced by heavy-ions (see details in Refs. [26, 27]).
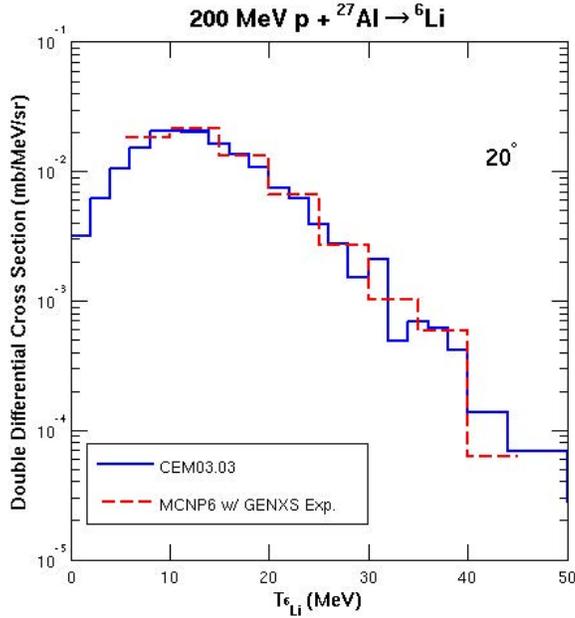

Figure 1: Comparison of emitted ^{6}Li double differential spectra for the reaction 200 MeV p + ^{27}Al, at an emission angle of 20°, calculated by MCNP6 with the extended GENXS (red dashed lines) and CEM03.03 used as a stand alone code (blue solid lines).

We recommend inclusion of the extended version of GENXS in all future official versions of

MCNP6, as an useful improvement to MCNP6.

5. Total Reaction Cross Sections in CEM/LAQGSM and MCNP6

Total reaction cross section models have a significant impact on the predictions and accuracy of spallation and transport codes. The latest version of the Cascade Exciton Model (CEM) [7, 8], as incorporated in the code CEM03.03 [8, 6] and MCNP6 [4], each use such cross sections for different purposes. While total reaction cross sections are used throughout the transport and spallation models, there are two main utilization. MCNP6 uses total reaction cross sections to determine where a reaction occurs (through the mean-free path length), and then with what nucleus the projectile interacts with, and lastly what type of interaction it is (inelastic or elastic). CEM uses total reaction cross sections as *inverse* cross sections to predict what the excited nucleus emits. Phenomenological approximations of total reaction cross sections are also used by CEM03.03 as the default option for normalization of all results in the case of reactions induced by protons and neutrons, when CEM03.03 is used as a stand alone code outside any transport codes; see details in Refs. [8, 6].

The current inverse cross sections used in the preequilibrium and evaporation stages of CEM are based on the Dostrovsky *et al.* model, published in 1959 [28]. Better total reaction (*inverse*) cross section models are available now [29]–[34] (see details and more references in [35]).

MCNP6 uses an update of the Barashenkov and Polanski (B&P) cross section model [33] as described briefly in [34, 36] to calculate the mean-free path length for neutrons, protons, and light fragments up to ^{4}He. It uses a parameterization by Mike James et al. [2] based on a geometric cross section for light fragments above ^{4}He. Implementing better cross section models in CEM and MCNP6 should yield improved results of particle spectra and total production cross sections, among other results.

Our recent results [35], upgrading the inverse cross section model in the preequilibrium stage of CEM, prove that this is, in fact, the case (see two examples in Fig. 2 and more details and other examples in [35, 37]).

As mentioned above, MCNP6 uses the updated Barashenkov and Polanski total reaction cross section systematics to simulate the mean-free path of neutrons, protons, and light fragments up to ^{4}He. It uses a parameterization based on a geometric cross section [2] for fragments heavier than ^{4}He. Possible direct improvement of MCNP6 may be obtained by replacing the Barashenkov and Polanski model with NASA systematics and by replacing the geometric cross section approach with the better NASA model. We recommend doing this in MCNP6 in the future and then checking with a number of test-problems as to how such improvement would change the MCNP6 results on both thin and thick targets irradiated with nucleons and heavy-ions.

Finally, let us note that in order to achieve better results, the authors of such known and widely used transport codes like PHITS, FLUKA, and GEANT4 studied and tried to improve recently, when possible, the total reactions cross sections used by their codes. Details on the total reaction cross section models used in PHITS, FLUKA and GEANT4 can be found in Ref. [35, 38, 39].
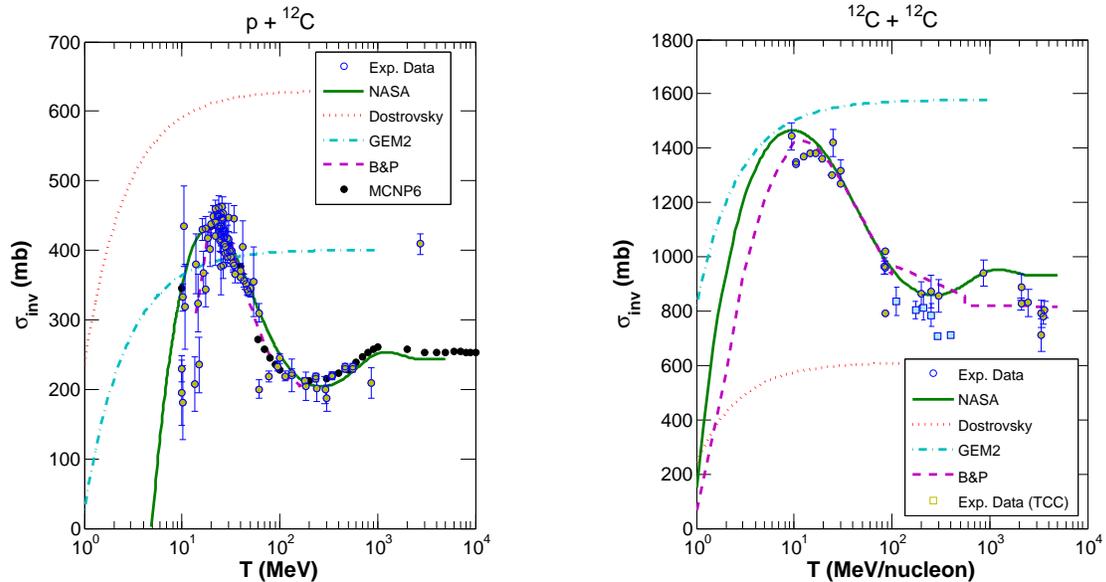
Figure 2: Reaction cross section for p + ^{12}C and ^{12}C + ^{12}C, as calculated by the NASA, Dostrovsky *et al.*, GEM2, and B&P models. The black dots are cross section calculations by MCNP6, and the circles and squares are experimental data. References to these experimental data and further details can be found in our recent paper [35].

6. The "F" version of CEM03.03/LAQGSM03.03 and MCNP6

During the past three years, serious efforts have been made at LANL to improve the CEM and LAQGSM event generators of MCNP6 in order to be able to describe production of energetic light fragments (LF) heavier than ^{4}He from various nuclear reactions; thus, improving the prediction capability of MCNP6 for the production of energetic heavy clusters (see, e.g., Refs. [27, 35, 37, 40, 41, 42, 43] and references therein). As a result, an improved version of CEM03.03 called "CEM03.03F" was developed, tested, and implemented in a local, working version of MCNP6, that we call "MCNP6-F" ("F" stand for "fragments", i.e., versions of the codes able to calculate emission of LF heavier than ^{4}He). The work on developing an "F" version of LAQGSM03.03 is still in progress, but the preliminary results we obtained so far [43] are encouraging; we hope to complete these efforts during 2015 and to test and implement LAQGSM03.03F in MCNP6-F during 2016.

As can be seen from Refs. [27, 35, 37, 40, 41, 42, 43] and references therein, the "F" versions of CEM03.03 and MCNP6 allow us to dramatically improve the prediction capability of our codes for the production of energetic LF heavier than ^{4}He from various reactions. Such processes are important for different applications, such as cosmic-ray-induced Single Event Upsets (SEUs), radiation protection, and cancer therapy with proton and heavy-ion beams, to name just a few.

Fig. 3 presents only one example of good results by CEM03.03F: We see that for this particular reaction, 480 MeV p + ^{nat}Ag → ^{6}Li, the standard version of CEM03.03 can not describe the high-energy tail of the ^{6}Li spectrum, while the "F" version, does this very well.

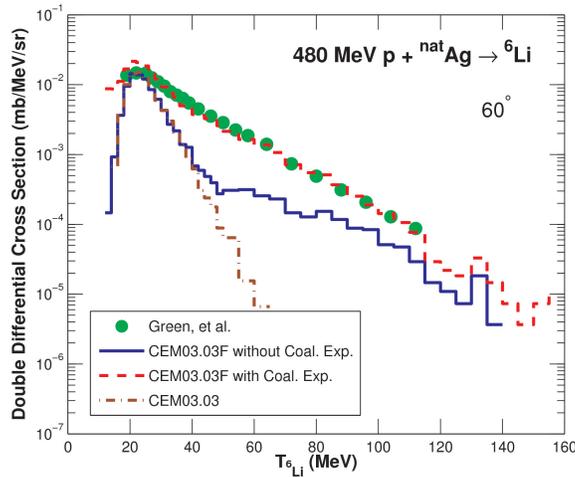Many more similar good results by CEM03.03F can be found in Refs. [27, 35, 37, 40, 41, 42, 43] and references therein.

Figure 3: Comparison of experimental results of the reaction 480 MeV p + ^{nat}Ag → ^{6}Li at 60° by Green *et al.* [44] (green circles) with simulations from the original CEM03.03 (brown dashed-dotted lines), CEM03.03F without coalescence expansion (blue solid lines), and the CEM03.03F with coalescence expansion (red dashed lines).

However, this does not yet mean that we can replace CEM03.03 with CEM03.03F in the production version of MCNP6, as we did with MCNP6-F (see Ref. [27]). To do so, we need to test initially CEM03.03F on as many as possible different reactions, including ones that we not used and tested while developing CEM03.03F, to make sure that CEM03.03F calculates such reactions "not worse" than the standard CEM03.03 does at present in MCNP6.

We have performed such a Validation and Verification (V&V) work of CEM03.03F, testing it on various reactions. Figs. 4 – 12 present examples of results from these V&V efforts. As we can see from Figs. 4 – 9, CEM03.03F describes these reactions at least as well as its precursor, the standard CEM03.03, providing meanwhile production of high-energetic LF heavier than ^{4}He absent in the later. Note that these reactions were not used in developing and "tuning" CEM03.03F, i.e., such results are actually pure predictions by CEM03.03F. It is worth mentioning that in some cases, CEM03.03F even shows some improvement in comparison with CEM03.03, like for fission yields from 800 MeV p + ^{197}Au (upper-left plot in Fig. 7) and for neutron-induced fission cross section of ^{209}Bi at energies around 100 MeV (lower-right plot in Fig. 11).

However, because CEM03.03F considers emission of LF at the preequilibrium stage, the mean values of A, Z, and excitation energy E^* of the fissioning nuclei differ a little from such values by CEM03.03. Therefore, it underestimates a little the fission cross sections of preactinide nuclei (see Figs. 10 and 11) and, respectively, the yields of fission fragments from such nuclei (see Fig. 12).

As was shown in Refs. [55, 63, 64], the main parameter that determines the fission cross sections calculated by CEM and LAQGSM for preactinide nuclei is the level-density parameter in the fission channel, a_f (or, more exactly, the ratio a_f/a_n, where a_n is the level-density parameter for neutron evaporation). Let us recall here that CEM and LAQGSM calculate now fission cross sections and fission fragment production with a modification of the Generalized
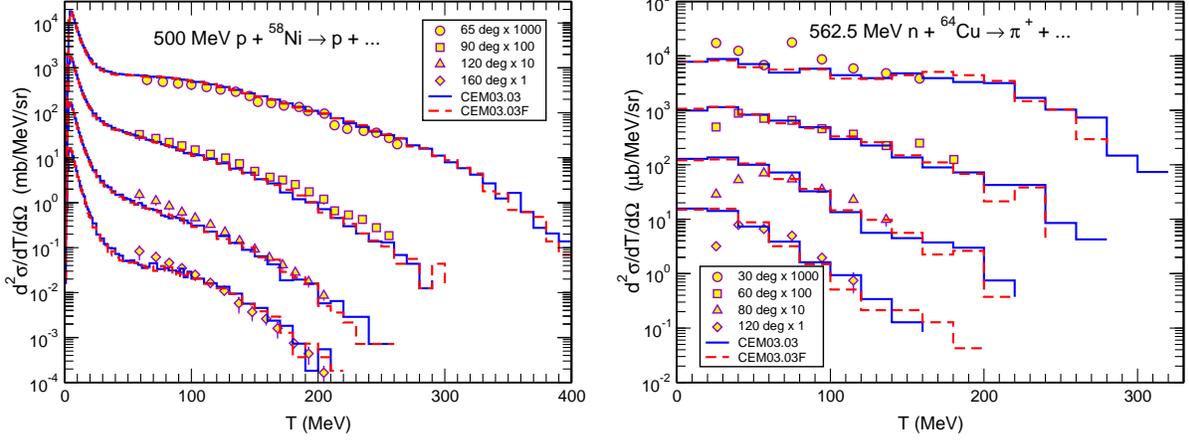
Figure 4: Comparison of experimental data by Roy, *et al.* [45] (symbols) with results by the standard CEM03.03 (blue solid lines) and new CEM03.03F (red dashed lines) for 500 MeV p + ^{58}Ni $\to$ p (left plot) and of data by Brooks, *et al.* [46] (symbols) with results by the unmodified CEM03.03 (blue solid lines) and CEM03.03F (red dashed lines) for 562.5 MeV n + ^{nat}Cu $\to$ π^+ (right plot).
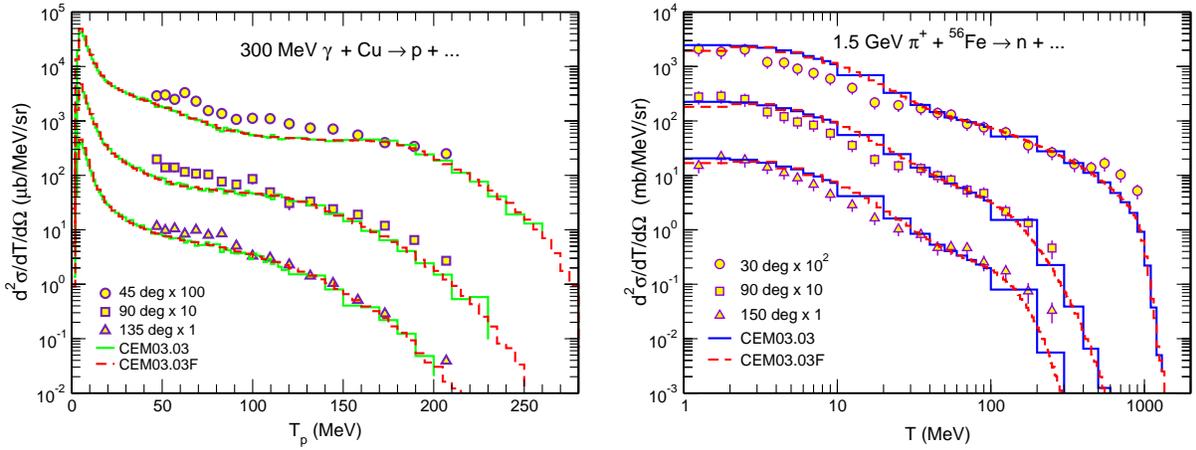
Figure 5: Comparison of experimental data by Schumacher, *et al.* [47] (filled symbols) with results by the standard CEM03.03 (green solid lines) and new CEM03.03F (red dashed lines) for 300 MeV γ+^{nat}Cu $\to$ p at 45°, 90°, and 135° (left plot) and with data by Nakamoto, *et al.* [48] (filled symbols) with results by the unmodified CEM03.03 (blue solid lines) and new CEM03.03F (red dashed lines) for 1500 MeV π^++ Fe $\to$ n at 30°, 90°, and 150° (right plot).

9
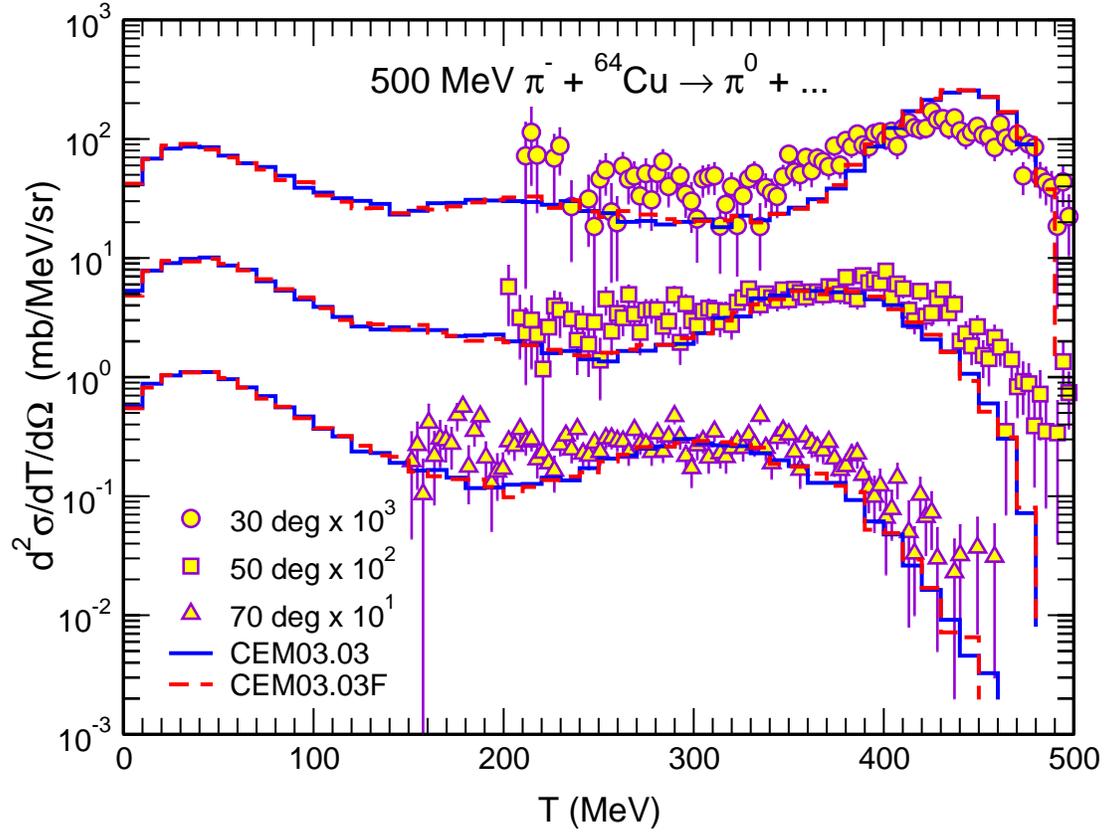
Figure 6: Comparison of experimental data [49, 50] (filled symbols) with results by the unmodified CEM03.03 (blue solid lines) and new CEM03.03F (red dashed lines) for 500 MeV π^-+^{64}Cu $\rightarrow \pi^0$ at 30°, 50°, and 70°.

Figure 7: Comparison of measured [51] mass and charge distributions of the product yields from the reaction 800 MeV p + ^{197}Au, and of the mean kinetic energy of these products, and the mass distributions of the cross sections for the production of thirteen elements with the charge Z from 20 to 80 (open symbols), with predicted results from the original CEM03.03 (solid lines) and the new CEM03.03F (dashed lines).

11
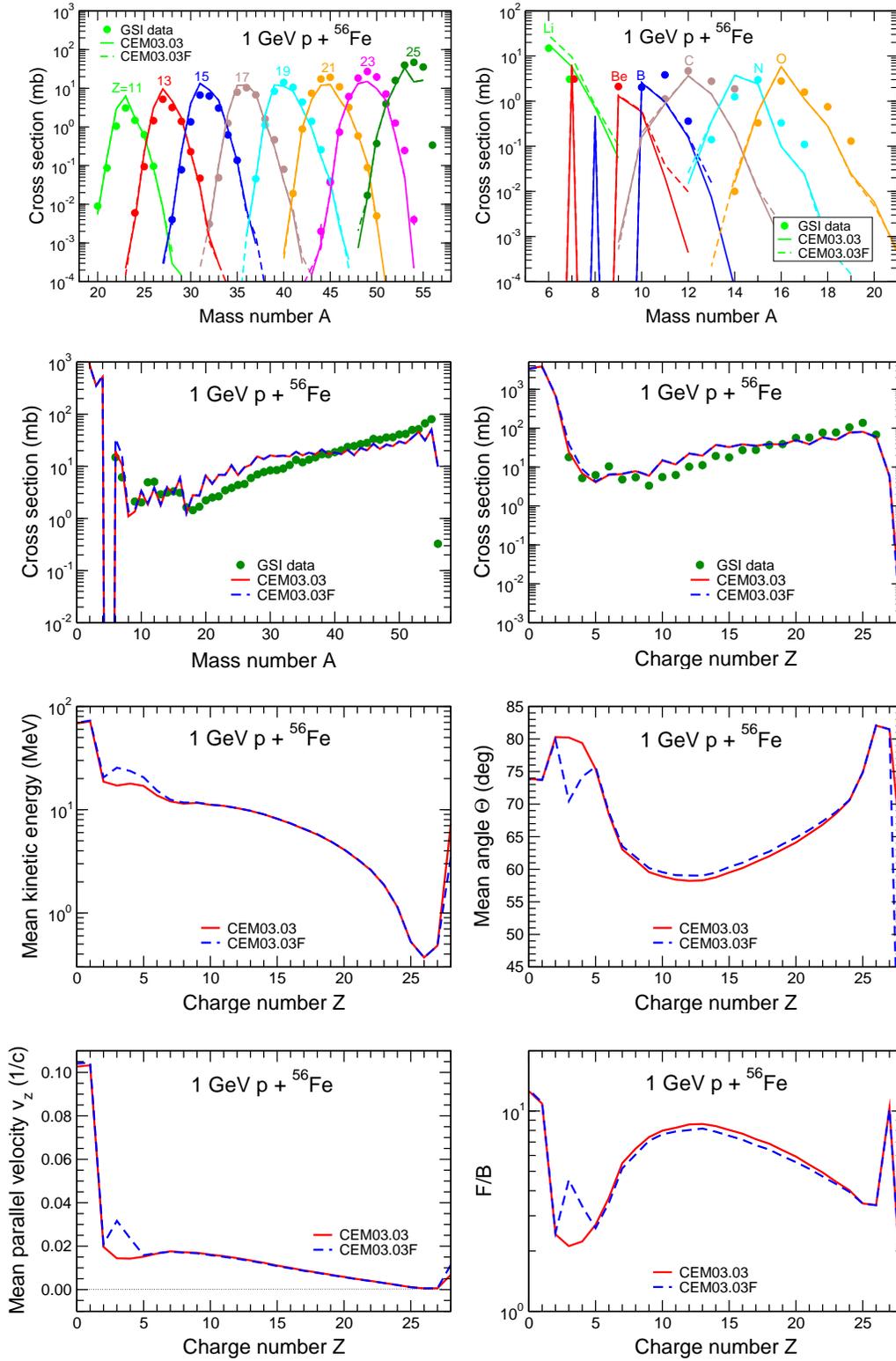
Figure 8: Experimental mass distributions of the yields of eight isotopes from Na to Mn [52] and of all light fragments from Li to O [53] from the reaction 1 GeV p + ^{56}Fe and the mass number- and charge-distributions of the product yield (color circles), compared with results from both CEM03.03 and CEM03.03F. Predictions of CEM03.03/F for the mean kinetic energy, mean production angle Θ, mean parallel velocity v_z, and of the F/B ratio of the forward product cross sections to the backward ones of all isotopes in the laboratory system are given as well.

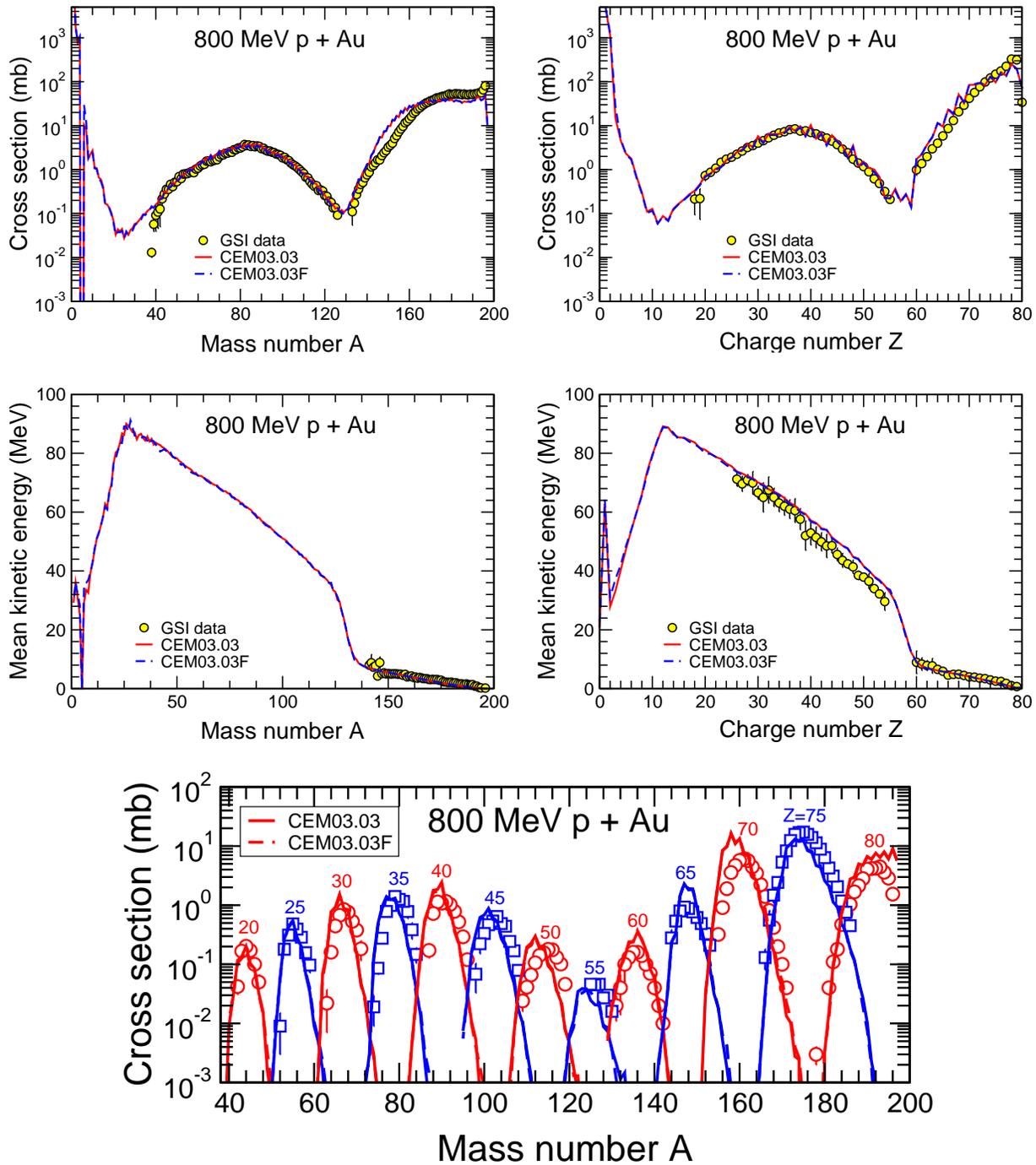Figure 9: Comparison of measured [54] mass and charge distributions of the product yields from the reaction 1000 MeV p + ^{nat}U, and of the mean kinetic energy of these products (color circles), with results by the unmodified CEM03.03 (red solid lines) and new CEM03.03F (blue dashed lines).
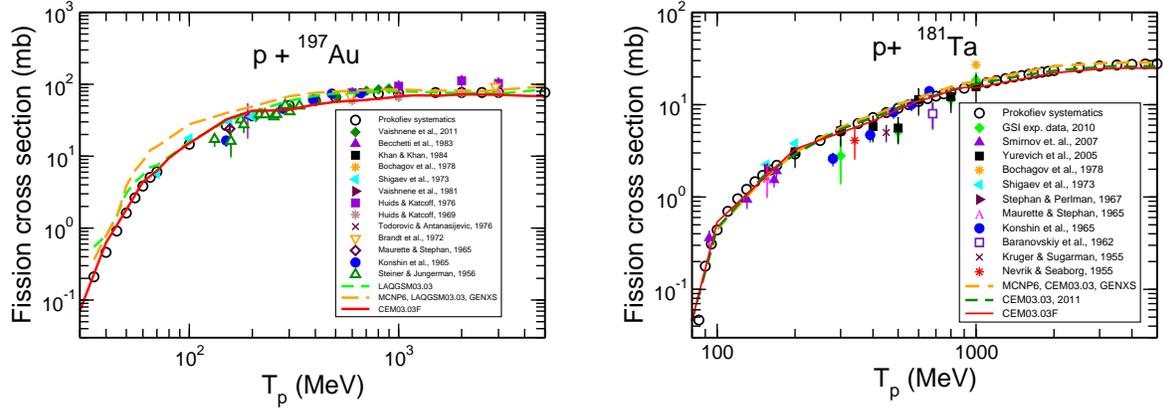
Figure 10: Comparison of experimental data for proton-induced fission cross sections of ^{197}Au and ^{181}Ta (symbols) with results by CEM03.03F (red lines) and with predictions by LAQGSM03.03 (for ^{197}Au), CEM03.03 (for ^{181}Ta), and by MCNP6 using LAQGSM03.03 (for ^{197}Au) and CEM03.03 (for ^{181}Ta) event-generators, as indicated. References to all experimental data used here and details on calculation fission cross sections by CEM and LAQGSM can be found in Ref. [55].

Figure 11: Comparison of experimental data for neutron-induced fission cross sections of ^{197}Au and ^{209}Bi (symbols) with results by CEM03.03F (dashed red lines) and with calculations with the standard CEM03.03 (solid lines). Experimental data for ^{197}Au are from Refs. [56, 57, 58] and ^{209}Bi, from [59, 60].
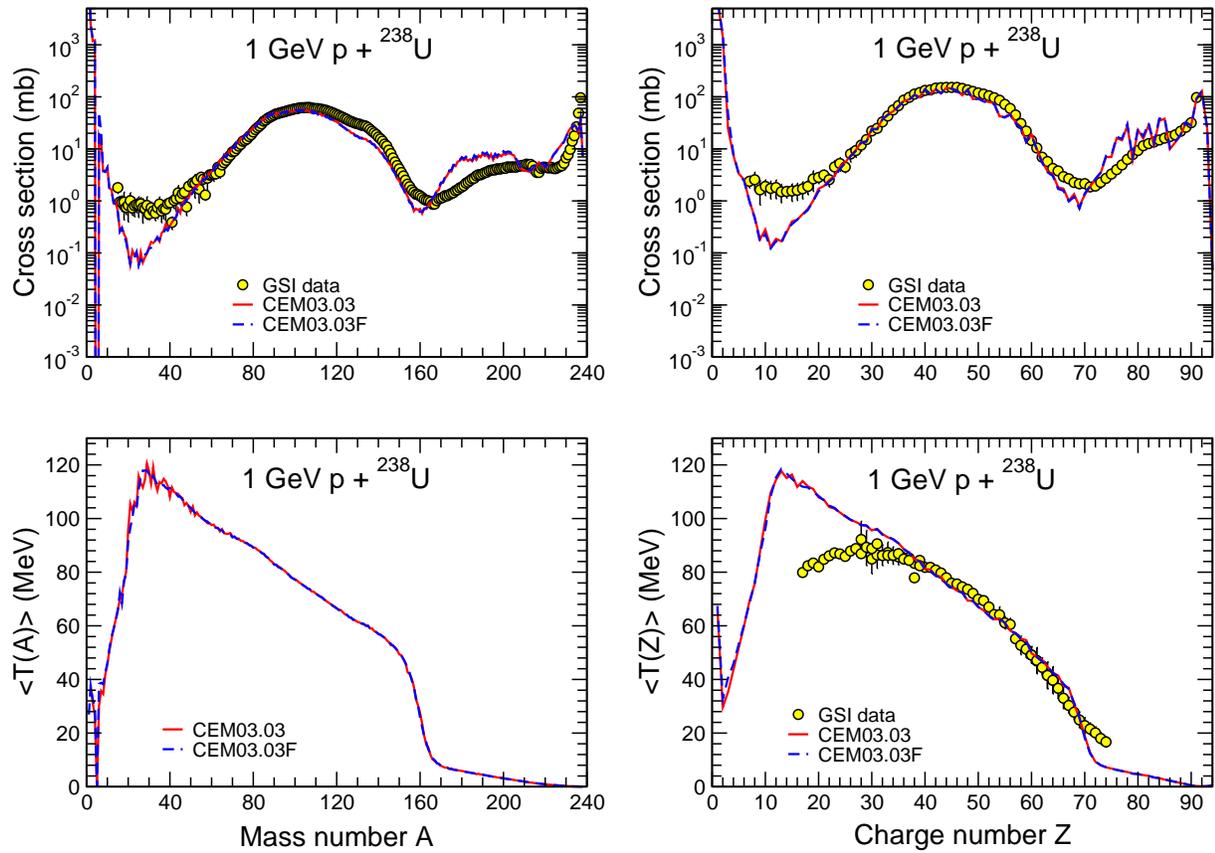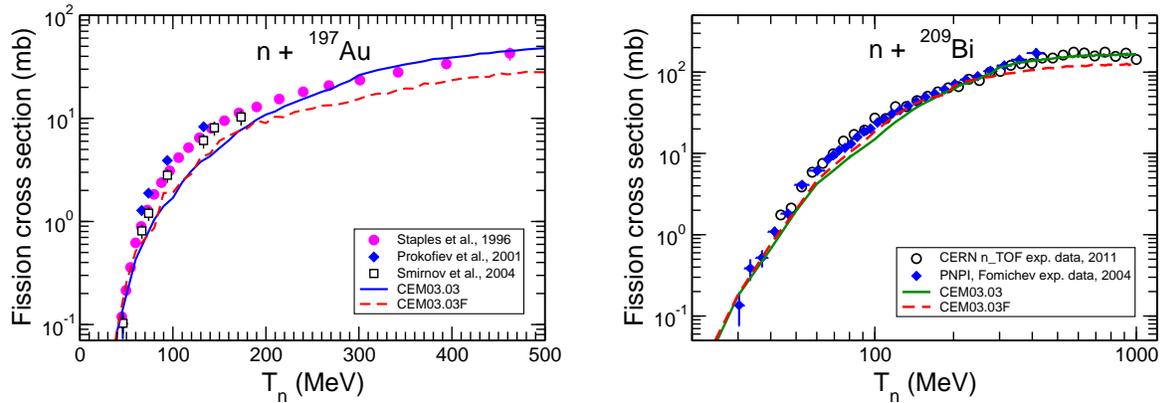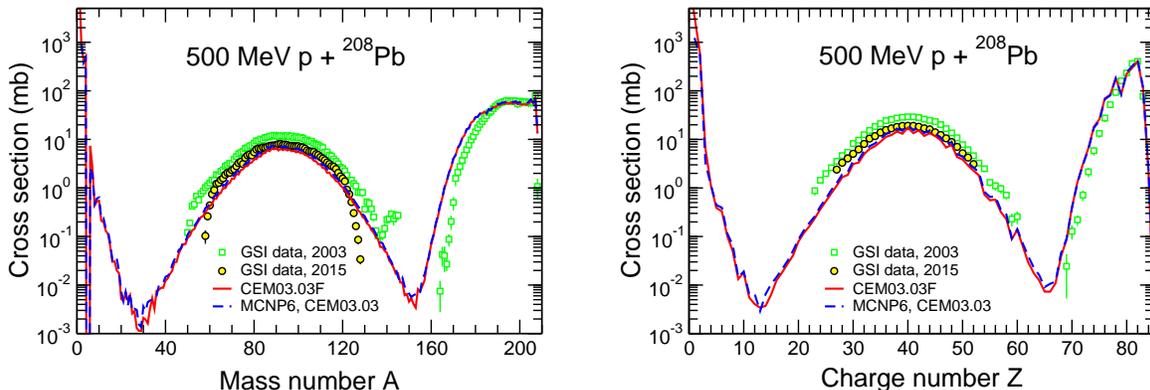
14

Figure 12: Comparison of measured [61, 62] mass and charge distributions of the product yields from the reaction 500 MeV p + ^{208}Pb (symbols) with results by CEM03.03F (solid red lines) and by MCNP6 using CEM03.03 (dashed blue lines).

Evaporation Model code GEM2 by Furihata [65]. GEM2 is an extension by Furihata of the Dostrovsky et al. [28, 16] evaporation model as implemented in LAHET [66] and includes up to 66 types of particles and fragments that can be evaporated from an excited compound nucleus plus a modification of the version of Atchison's fission model [17] used in LAHET. It was found [63] that if we were to merge GEM2 with the latest version of the CEM we had at that time, or with LAQGSM, without any modifications, the new code would not correctly describe the fission cross sections. This is because Atchison fitted the parameters of his fission model when it was coupled with the Bertini Intra-Nuclear Cascade (INC) [14] which differs from our INC, and did not model preequilibrium emission. Therefore, the distributions of fissioning nuclei in A, Z, and excitation energy E^* simulated by Atchison differ significantly of the distributions we get; as a consequence, all the fission characteristics are also different. Similarly, Furihata used GEM2 coupled either with the Bertini INC [14] or with the ISABEL [20] INC code, which also differs from our INC, and also did not include preequilibrium particle emission. Thus the parameters adjusted by Furihata to work the best with her INC will not work well for ours. To get a good description of fission cross sections (and fission-fragment yields) we had to modify at least two parameters in GEM2 (see details in [63]). This problem was solved both for CEM2k+GEM2 and LAQGSM+GEM2 in the work [64], and for the latest, "03.03", versions of CEM and LAQGSM, in Ref. [55].

To improve in CEM03.03F the description of fission cross section, and of the yield of fission fragments, a refitting of the a_f/a_n parameter (and of the $C(Z)$ parameter, in the case of actinide nuclei) would be desirable. A similar "fine-tuning" of these parameter would be also necessary in the "F" version of LAQGSM03.03 [43], when it is completed, before its implementation in the "F" version of MCNP6. All details on the RAL and GEM2 codes and all formulas used by them to calculate fission cross sections can be found in Refs. [17, 65]; all details on their modifications in CEM/LAQGSM are described in Refs. [64, 55].

7. Multifragmentation and Fission-Like Binary Decay in CEM/LAQGSM

Generally, the latest versions of CEM and LAQGSM, CEM03.03 and LAQGSM03.03, de-

15

scribe nuclear reactions much better than their predecessors and most of other similar codes available to the nuclear physics community. They have been benchmark-ed on a variety of particle-particle, particle-nucleus, and nucleus-nucleus reactions at energies from 10 MeV to 800 GeV per nucleon, and have been incorporated into and are used as event generators in the transport codes MCNP6, MARS, and MCNPX. The recent "F" version of them, mentioned in the previous section, is even better, as it allows us to describe emission of energetic LF from practically arbitrary reactions, a capability not supported yet at present by any other codes, to the best of our knowledge.

Nevertheless, these versions of CEM/LAQGSM codes fail to reproduce correctly production of fission-like heavy fragments from reactions with medium and light nuclei (see Figs. 13 and 14). Such nuclear targets are considered too light to fission in conventional codes (including GEM2 and all models currently employed in large-scale transport codes). Similarly, the fragments are too light to be produced as spallation residues and too heavy to be produced via standard evaporation and/or preequilibrium models, or via coalescence.
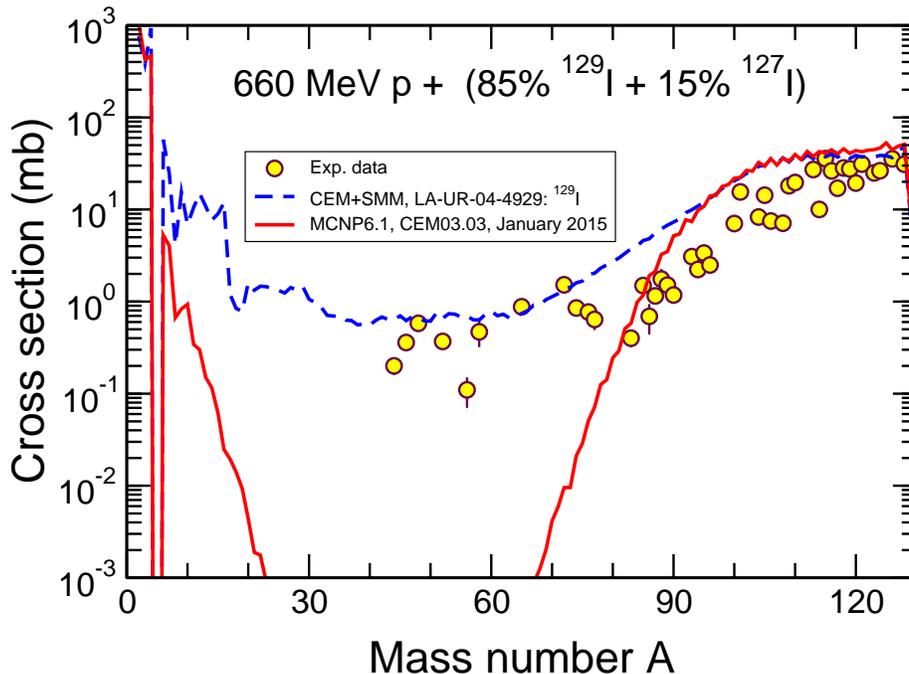
Figure 13: Comparison of measured [67] mass distributions of product yields from 660 MeV p + ^{129}I (85% ^{129}I + 15%^{127}I) compared with our recent calculations by MCNP6 using CEM03.03 (solid red line), and with our old results by the CEM03.S1 (i.e., CEM03.01 [68] merged with SMM [69]) published in Ref. [70] (dashed blue line).

One way to approach this problem is to describe the fast part of a nuclear reaction with an IntraNuclear Cascade model (INC) followed by preequilibrium emission of particles during the equilibration of the excited residual nucleus. At this point, one would employ a fission-like sequential-binary-decay model, like the well-known code GEMINI by Charity [71], to describe the compound nuclear decay. In our case, this means separately merging CEM and LAQGSM

with GEMINI. Actually, we already have done so more than a decade ago, with the versions of CEM and LAQGSM we had at that time, and some preliminary results from that merged versions of our codes can be found, e.g., in Refs. [67, 70, 72, 73].
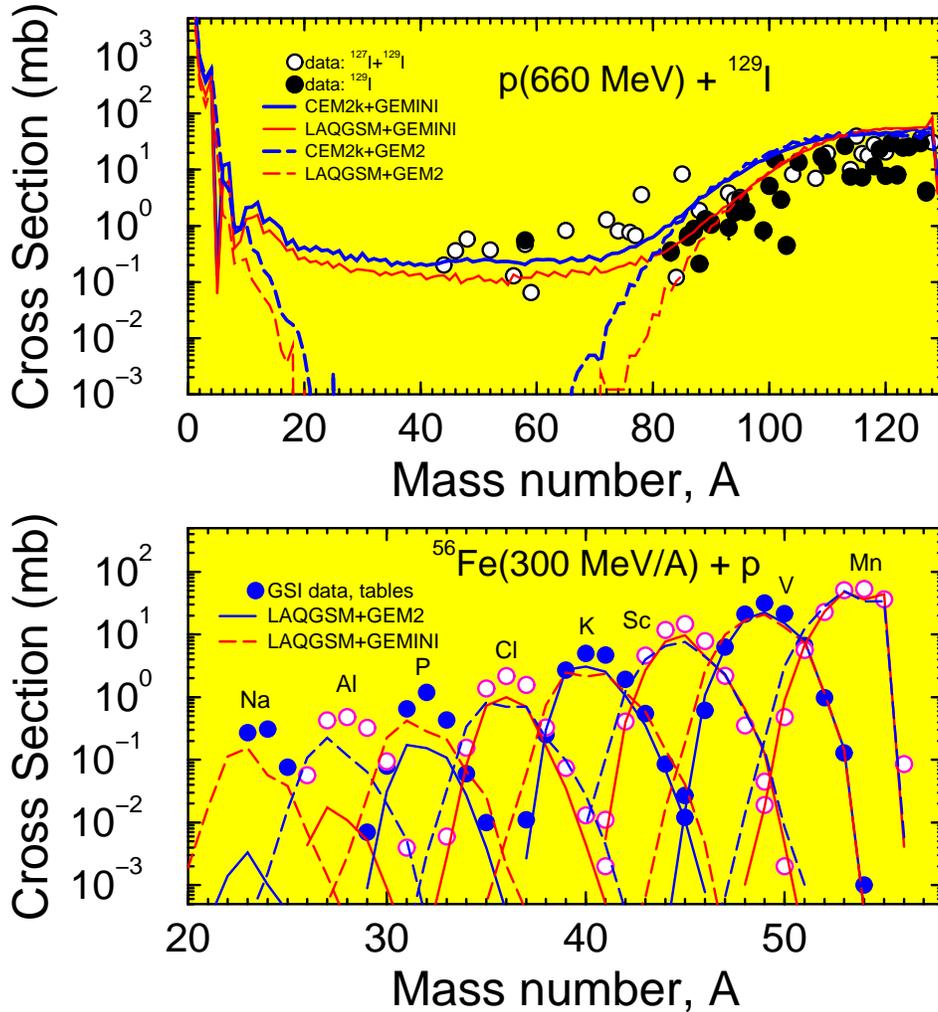
Figure 14: Top plot: Experimental data on 660 MeV p + ^{129}I (and ^{127}I + ^{129}I) [67] compared with mass distributions of products predicted by CEM2k and LAQGSM merged with GEM2 (dashed lines) and GEMINI (solid lines), as indicated. Bottom plot: Experimental [52] mass distributions of the yields of eight isotopes from Mn to Na produced in the reaction 300 MeV/A ^{56}Fe + p compared with LAQGSM+GEM2 (solid lines) and LAQGSM+GEMINI (dashed lines) results. $t\_delay = 0.1$ and $sig\_delay = 0.1$ are used in GEMINI to calculate both these reactions.

Another way to address this problem is to implement in CEM and LAQGSM the Statistical Multifragmentation Model (SMM) by Botvina et $al.$ [69]. Thus, we would consider multi-fragmentation as a mode competitive to evaporation of particles and light fragments, when the excitation energy E^* of a compound nucleus produced after the preequilibrium stage of a reaction is above a certain value, E^*_{tr}, e.g., $E^*_{tr} = 2 \times A$ MeV, as we did in the "S" versions of CEM03.01 and LAQGSM03.01 (see, e.g., Refs. [72, 67, 70, 73]). This way, we have produced the "S" version of our codes ("S" stands for SMM), CEM03.S1 and LAQGSM03.S1.
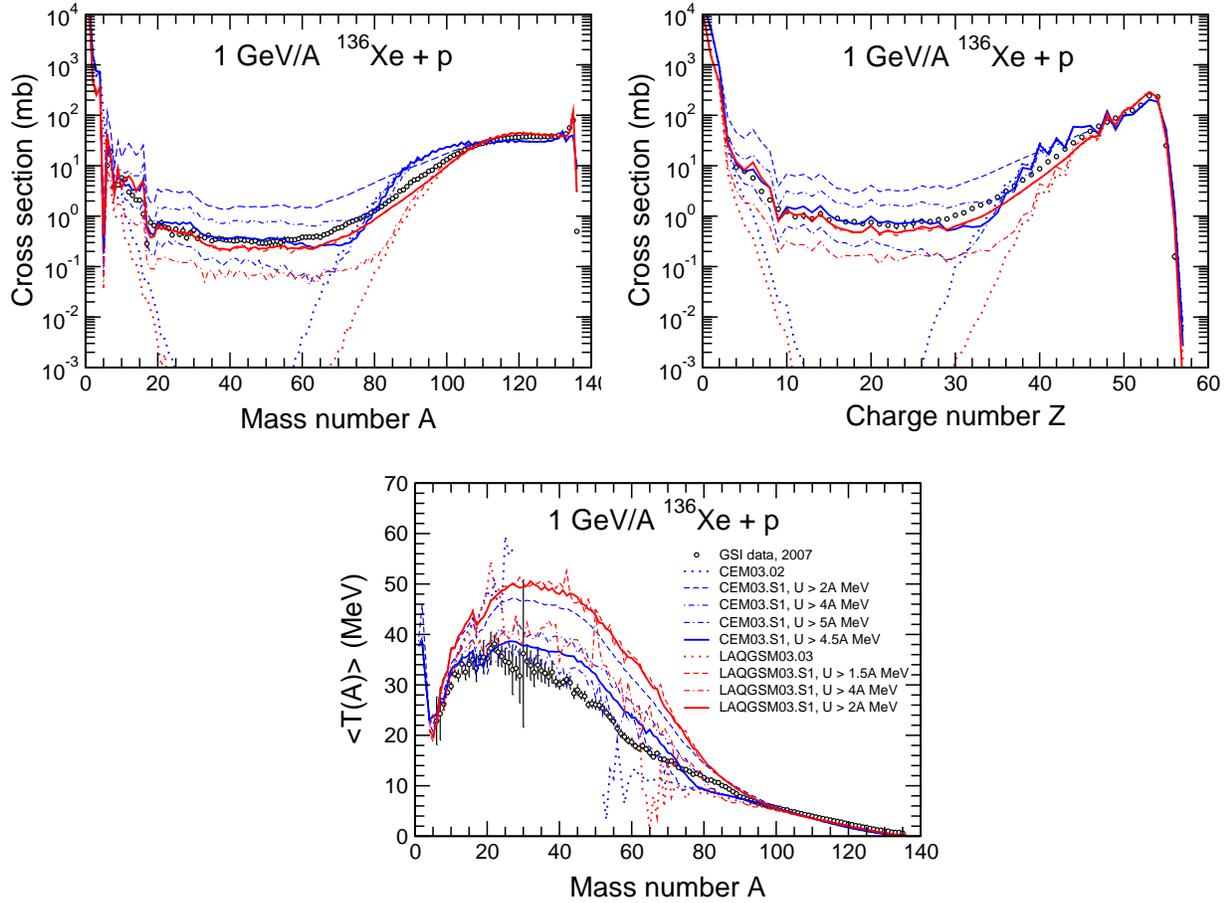
Figure 15: Mass- and charge-product yield distributions and mean kinetic energy of all products as functions of the product mass number from the reaction 1 GeV/nucleon ^{136}Xe + p [74] (open circles) measured at GSI compared with calculations by the standard CEM03.03 and LAQGSM03.03 (dotted lines), as well as by their "S" versions (solid and dot-dashed lines) for different values of the excitations energy E^*_{tr} of the nuclei produced after the preequilibrium stage of reactions above which we start to consider multifragmentation as a competitive reaction mechanism, namely, at E^*_{tr} (shown in legend as U)> 2, 4, 4.5, and 5 MeV/nucleon in the case of CEM03.S1, and $E^*_{tr} > 1.5$, 2, and 4 MeV/nucleon for LAQGSM03.S1, as indicated.

As of today, neither the "S" nor the "G" versions of CEM and LAQGSM have been implemented in MCNP6/X, and for serious reasons: Just as any other theoretical models, SMM [69] and GEMINI [71] have their own parameters, and some of them affect drastically the final results. The most sensitive parameter of SMM that affects the calculated products from nuclear reactions is the "transaction" energy, E^*_{tr} (or the temperature) of the excited nucleus, when the nuclear reaction mechanism changes from evaporation (at lower energies) to multifragmentation (at excitation energies above E^*_{tr}). Following advise by the main author of SMM, Dr. A. Botvina, we implemented in the "S" versions of our codes [72] the value $E^*_{tr} = 2$ MeV/nucleon. This is, when after the preequilibrium stage of a reaction $E^* > E^*_{tr} = 2 \times A$ MeV, we "activate" SMM to calculate multifragmentation in the 03.S1 codes; the competitive evaporation process are calculated then also with a version of the evaporation model by Botvina *et al.* from SMM, rather than using GEM2, as we do always in the standard 03.01 versions and in 03.S1 when

$E^* \leq 2 \times A$ MeV and SMM is not invoked.
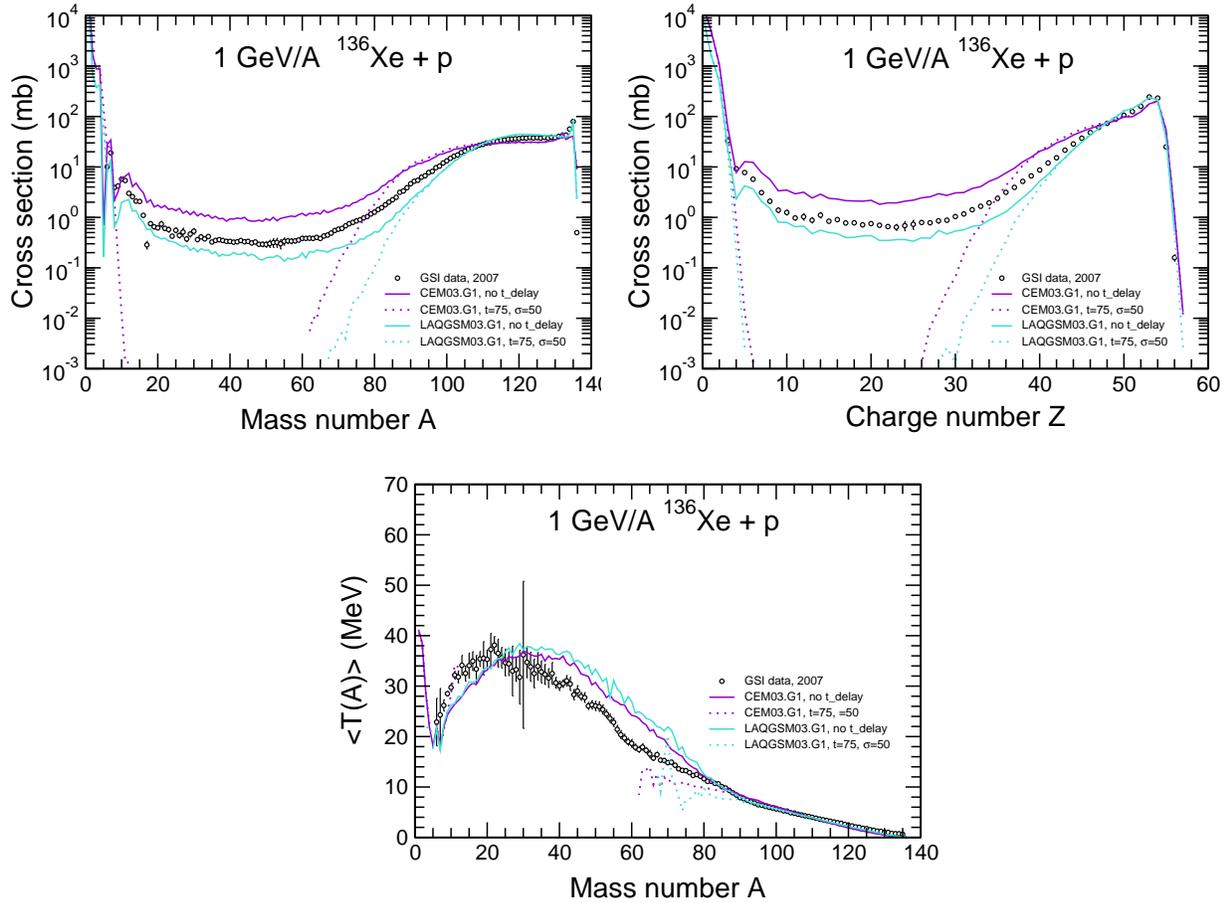
Figure 16: The same experimental data [74] as in previous figure, but compared with results of calculations by CEM03.G1 (violet lines) and LAQGSM03.G1 (turquoise lines), as indicated.

Fig. 15 shows only one example of a reaction calculated with the "S" version of CEM and LAQGSM, when the "default" value $E^*_{tr} = 2 \times A$ MeV does not work well for our codes: We see that the best agreement of results by LAQGSM03.S1 (solid red lines in Fig. 15) with the GSI data [74] was achieved for $E^*_{tr} = 2$ MeV/nucleon, just as Dr. Botvina suggested. But in the case of CEM03.S1 (solid blue lines in Fig. 15), we got the best agreement with the data for a higher energy, namely $E^*_{tr} = 4.5$ MeV/nucleon. Note that for several other reactions we studied with the "S" versions of our codes, we got slightly different "best" values for E^*_{tr}. Let us also note that the fact that we get different "best" values of E^*_{tr} when we need to "activate" multifragmentation as a competition to the simple evaporation mechanism in different codes is not contradictory and does imply something physical: The INC of CEM is completely different from the one of LAQGSM, therefore the mean mass $< A >$ and charge number $< Z >$ of residual nuclei produced after the preequilibrium stage of a reaction with an excitation E^* higher than a certain values, *e.g.*, $E^*_{tr} = 2$ MeV/nucleon, should be also different, as should be the distributions of such nuclei with respect to their E^*. This results in different fragments produced via multifragmentation from the same reaction as predicted by CEM03.S1 and LAQGSM03.S1. In other words, in order to describe as well as possible reactions simulated with the "S" versions of CEM and LAQGSM, the values of E^*_{tr} must be fine-tuned separately in

both event-generators, for as many as possible various nuclear reactions, at different energies. This is a time consuming task requiring a lot of effort, man-power, and funding: It is not an easy and interesting job that could be done during the evenings or weekends, as a hobby, as we actually performed many recent improvements to our codes (e.g., one of the main co-author of both CEM and LAQGSM, Dr. K. K. Gudima, was funded last time by LANL for his efforts only in 2004, i.e., 11 years ago; all his later work on CEM/LAQGSM development was done by him only as a "hobby", without any funding from our side). So far, our sponsors have not been interested in such an improvement of MCNP6, though it would affect significantly the predictions by MCNP6 for applications involving intermediate-mass fragment produced from reactions on medium and heavy nuclei.

GEMINI [71] also has its own parameters, that affect seriously the results: *t_delay* and *sig_delay* being ones of the most "sensitive". Our experience shows that in order to get good agreement of the "G" versions of our codes with available experimental data, we need to tune these two parameter in GEMINI. Unfortunately, we again got different "best" values for different reactions (see e.g., Fig. 16 above, and, especially, Fig. 5 in Ref. [75]). This means, before implementing the "G" versions of our CEM and LAQGSM event generators in a production version of MCNP6, we have first to fine-tune these two parameters of GEMINI on as many as possible nuclear reactions, at different energies. This would require again significant effort, man-power, and funding.

The situation becomes even more unclear if we compare the results shown in Figs. 15 and 16: The same data [74] can be reproduced either with the "S" versions of our codes, or, even a little better, with the "G" versions of our codes, without considering multifragmentation at all. In other words, it is not clear which are the "real" mechanisms of nuclear reactions involved in intermediate-mass fragment production from this reaction: multifragmentation or fission-like binary decay?

We believe that both these mechanisms are "real" and should be accounted by our codes. True, their contributions may be different in different regions of excitation energies of excited nuclei (and also depend on their mass- and charge-numbers), as illustrated in Fig. 17, adopted from Ref. [76], and used now in our MCNP6 classes.

We strongly suggest spending the needed efforts and funds to add both "S" and "G" mechanisms of nuclear reactions into the MCNP6 event generators, as discussed above. Note that a simplified scheme of accounting different de-excitation models for excited compound nuclei, including the "S" and "G" mechanisms discussed above, similar to the one shown in Fig. 17, was realized recently in ABLA07 [77], and merged successfully thereafter with the Liège INC code INCL4.5 [78]. However, we can not rely in MCNP6 on ABLA07 for several reasons: First, we can not merge ABLA07 with our different MCNP6 event-generators, without a significant modification of ABLA07, which is not allowed by its authors. Second, because the authors of ABLA07 do not allow anybody to modify their code, even the authors of the last version of the Liège INC code, INCL++, [79], could not use ABLA07. When INCL++ was implemented in the transport code GEANT4, they have to use other de-excitation models together with INCL++, as ABLA07 was not available to them for such a work (see details in [79]). Finally, I believe that any serious transport code should rely first of all on models and event-generators developed locally, at its own laboratory, so that when needed, such models can be improved and modified, without relying much on codes received as "black boxes" from other other places/countries. As far as I know, such a policy is followed practically by all serious production codes, in all countries; I suggest to do the same in MCNP6.
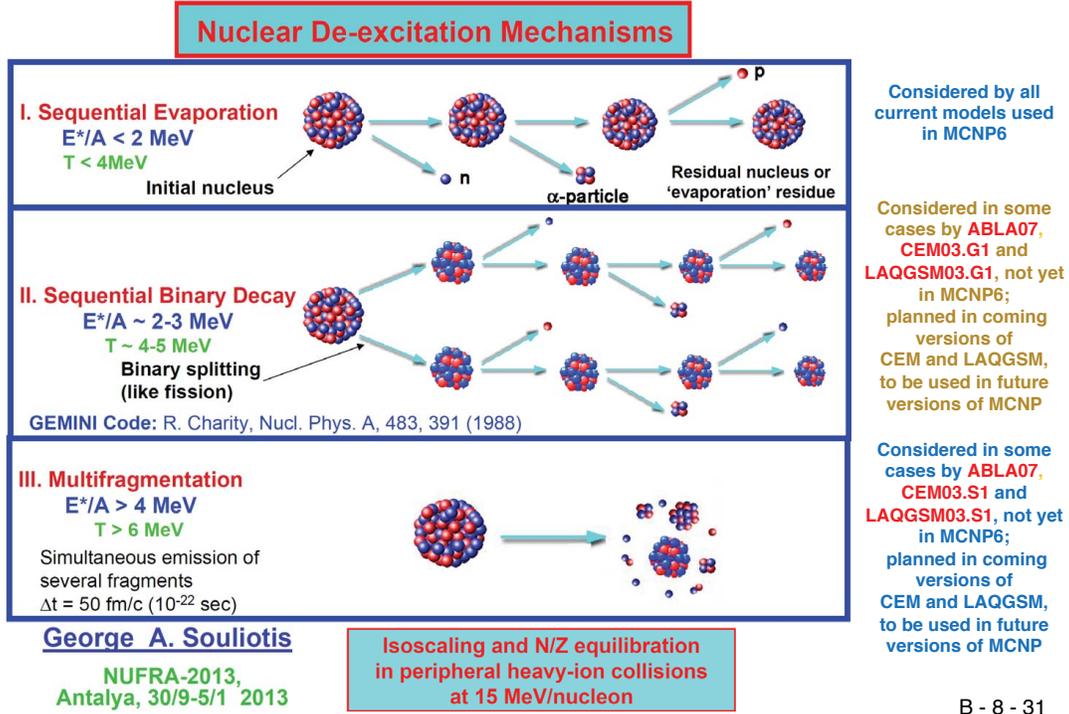
Figure 17: Different de-excitation mechanisms considered/(planned for future) by MCNP6, as illustrated by George Soulios in Ref. [76] and used now in our MCNP6 classes.

8. Evaporation and Fission Models in CEM/LAQGSM

As mentioned above, CEM03.03 and LAQGSM03.03 use the Generalized Evaporation Model code GEM2 by Furihata [65] to simulate the evaporation and fission stages of nuclear reactions. GEM2 is an extension by Furihata of the Dostrovsky et al. [28, 16] evaporation model as implemented in LAHET [66], often referred simply as "Dresner"; it includes up to 66 types of particles and fragments that can be evaporated from an excited compound nucleus, plus a modification of the version of Atchison's fission model [17] used in LAHET, referred often in the literature as "RAL" fission model.

GEM2 is a real step forward in simulating such reactions in comparison with the initial Dresner evaporation and RAL fission models, providing better agreement with experimental data for many reactions, and allowing evaporating 66 types of particles and LF, up to ^{28}Mg. However, in some aspects, from a theoretical point of view, Dr. Furihata did not extend too much the initial Dresner evaporation and RAL fission models; therefore, her GEM2 code has a number of quite rough approximations and does not provide reliable results for some reactions.

As examples, we list below only a few problems in GEM2 that should be addressed to improve the simulation of evaporation/fission reactions by GEM2:

1) *Inverse cross sections.* In Sec. 6, we discussed the "F" version of the CEM/LAQGSM codes we developed recently (see e.g., [27, 35, 37, 40, 41, 42, 43] and references therein). One of the improvements we did in the "F" version of our codes was replacing in the preequilibrium model the use of the old inverse cross section approximation by Dostrovsky et al. [28] with newer and better approaches developed at NASA and by Kalbach [29] – [32]. In "F", we did this only for the preequilibrium stage of reactions, but not for evaporation. Many results obtained recently with "F", show that improvement of the inverse cross sections at the evaporation stage, in GEM2, would increase significantly the agreement with experimental data of the evaporation peaks of spectra simulated in our codes by GEM2 (see e.g., [27, 35, 37, 40, 41, 42, 43]).

2) *Fission calculation by GEM2.* The initial GEM2 [65] calculates fission cross sections and production of fission fragments only for nuclei with charge number $Z \geq 70$, using a phenomenological model based on RAL [17]. In CEM and LAQGSM, we extended the calculations of fission reactions with GEM2 down to $Z = 65$ and made a few needed adjustments to use GEM2 by our codes, but we still do not consider fission of nuclei with $Z < 65$.

3) *Angular momentum neglected by GEM2.* GEM2 does not consider at all angular momentum of excited nuclei undergoing evaporation or/and fission. For particle-induced high-energy reactions on not too heavy nuclei, such an approximation may be good enough for many problems, as angular momentum of compound nuclei in such reactions are not expected to be very high, while their excitation energy are expected to be much larger than the rotation energy of the compound nuclei. But for reactions on heavy nuclei, especially induced by nuclei, such an approximation may be too bad, as the angular momentum of compound nuclei in such reactions may reach very high values. In such cases, the rotation energy of compound nuclei may be of the same order of magnitude as their internal excitation energy. Neglecting the angular momentum in such cases may cause poor results both for the evaporation and fission reactions.

4) *Phenomenological nature of the fission model in GEM2.* As mentioned above, GEM2 describes fission cross sections with an improved version of the RAL fission model [17], which relies more on available experimental data rather than on theory of fission, being therefore quite phenomenological. For this reason, for instance, we need to fine-tune at least two parameters in the fission models of GEM2, when we change the INC, or preequilibrium, or evaporation stages of our models, leading to a change of the mean $< A >, < Z >$, and $< E^* >$ of fissioning nuclei (see the discussion at the end of Sec. 6 about a_f/a_n and $C(Z)$ parameters in GEM2).

5) *γ emission at the evaporation/fission stages of reactions.* CEM03.03 and LAQGSM03.03, just like all other high-energy event-generators used at present in MCNP6, do not describe emission of γ's from residual nuclei with an excitation energy below the threshold of particle evaporation, i.e. a few MeV. (They neglect also emission of γ's with higher energy, as a competitor to evaporation and preequilibrium-particle emission, since the cross sections of such processes are insignificant compared to those of particle emission.) When using CEM03.03, Bertini, and ISABEL event generators in MCNP6, they are supplemented by a module with the same function as the **PHT** code from LAHET [66], which describes the cooling of such excited nuclei via γ emission. PTH is semi-phenomenological and accounts emission of γ's only after evaporation. It does not account competition of γ emission with evaporation of particles and LF, therefore, it does not provide any types of correlations of such γ's with other particles. However, recently, importance of correlations in energy and angle of the prompt neutrons and gamma rays emitted in the fission process for differential and integral experimental data are discussed. Recent efforts are made to account such correlations in MCNP6 with new

models/codes, like FREYA and CGMF (see, e.g., [80] and references therein) to be used at low energies as "new event generators in MCNP6" to simulate fission reactions, when correlations are needed. Let us mention that there are no big problems with accounting for γ-emission during the evaporation/fission stages of reaction in our CEM and LAQGSM event generators: Simply we need to calculate the width Γ_γ of γ-emission during the evaporation (and maybe also during the preequilibrium) stages of reactions, and to simulate emission of gammas in competition with other particles and LF, using the same Monte Carlo method and the same technique as we do now for emission of particles and fragments. Actually, two decades ago we had a version of CEM accounting for emission of gammas [81] at both evaporation and preequilibrium stages of reactions. But adding emission of gammas in that version of CEM resulted in a significant increase of the computing time. As we were not interested in γ-emission in our earlier work, to save computing time, we did not consider γ-emission in all our subsequent versions of CEM (and LAQGSM). But, taking into account the current interest in $\gamma - \gamma$ and $\gamma - n$ correlations for some applications involving fission reactions, if we find funding to improve the evaporation/fission models in CEM/LAQGSM, we could add γ-emission in our codes. To not increase the computing time, we can adopt as the "default" option not using γ-emission in our codes. But we can easily activate the γ-emission possibility in our codes, when needed, with an input parameter.

As can be seen from Fig. 18, for the reaction 500 MeV/A ^{208}Pb + p measured in inverse kinematics at GSI [61, 62], CEM03.03F as well as MCNP6 using the CEM03.03 event generator predict not only a little too low fission fragment yields, as observed above in Fig. 12, but also not a good A-distribution for all measured fission fragments: The calculated distributions are not wide enough, and are shifted a little to the left, i.e., to the neutron-deficient region of products.

Fig. 19 shows that our models have also some problems predicting a good description of some spallation products from this reaction, measured in Ref. [61]: We see that the "F" version of CEM03.03 describes a little better that the standard CEM03.03 the yields of neutron-rich spallation products; however, for some reactions, both models overestimate the production of isotopes in the maximum of their distribution, like in the case of Os, Re, W, Ta, and Hf isotopes. We see also a big discrepancy for the production of neutron-deficient Au isotopes, which we do not understand so far.

Let us note that serious problems with a good description of this reaction were met previously with other codes. So, from my numerous discussions with Dr. Sylvie Leray of CEA Saclay, a coauthor of measurements published in Ref. [61] and of several versions of INCL, I learned that the authors of that experiment met some real problems in a proper description of their data with early versions of INCL + ABLA and with several other codes available to them. Some examples of such problems can by seen in figures published in Ref. [61]. We met this problem for the same reaction, but at an incident energy of 1 GeV, with an older version of CEM, CEM97. When solving it, we developed a newer version of CEM, CEM2k (see details and further references in [82]).

Only in the very recent Ref. [62], using the 4.6 version of INCL, INCL4.6, [83] merged with ABLA07 [77], it was possible to get good agreement with practically all measured fission data for this reaction. Replacing in MCNP6 the current old versions of INCL [21] and ABLA [22] with their newer and better versions INCL4.6 [83] and ABLA07 [77] would be very useful to MCNP6, helping us to get better results for reactions where the INCL4.6+ABLA07 package was developed and fitted. However, even using INCL4.6+ABLA07 in MCNP6 would not solve all problems, as INCL4.6 does not describe photonuclear reactions, and fission induced by stopped
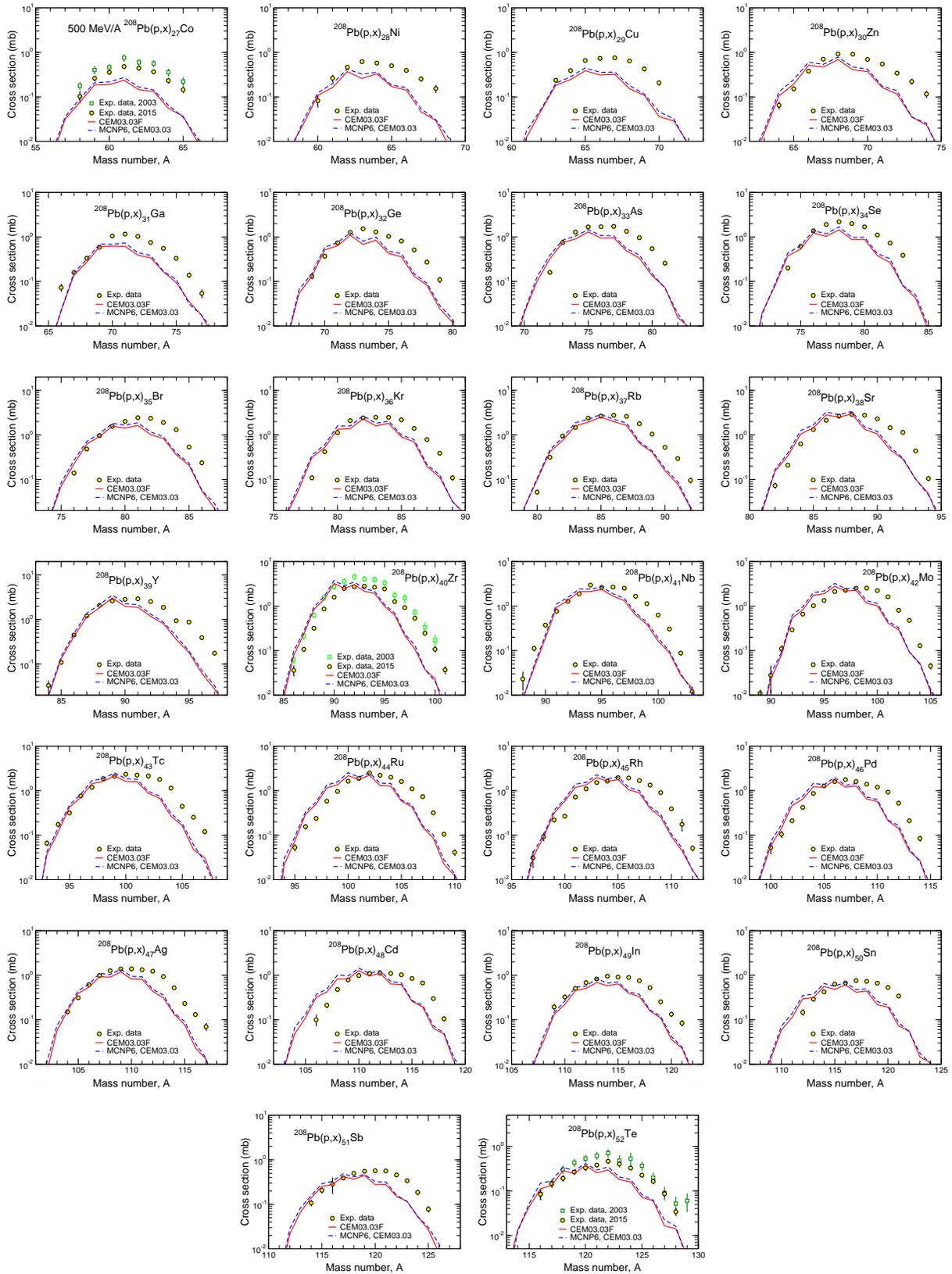
Figure 18: Experimental mass distributions of fission fragment yields, from Co to Te, from 500 MeV/A ^{208}Pb + p measured recently in Ref. [62] (circles) compared with CEM03.03F results and with calculations by MCNP6 using CEM03.03. For comparison, for Co, Zr, and Te, the older experimental data from [61] are also shown with green squares.
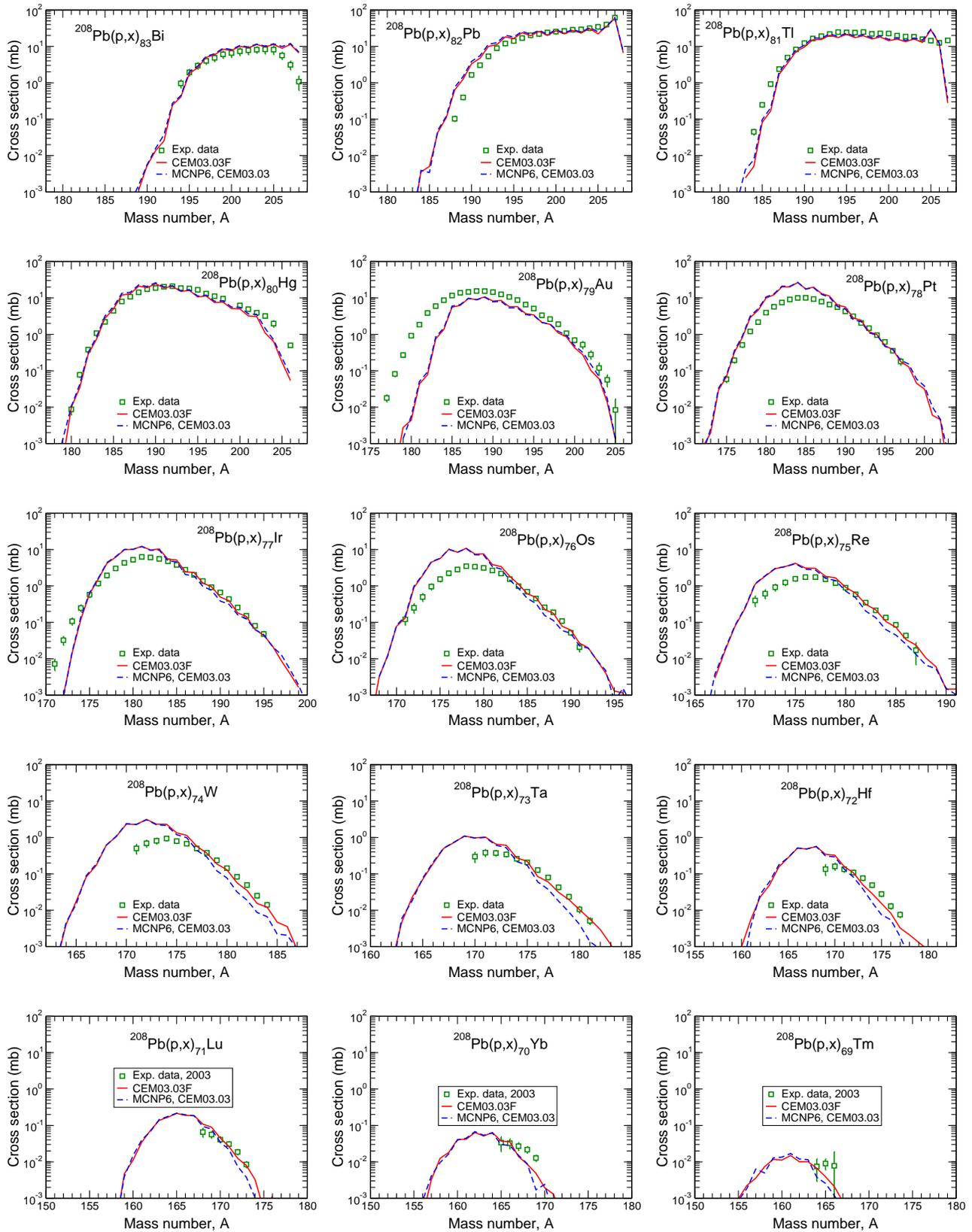
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Figure 19: Experimental mass distributions of spallation product yields, from Tm to Bi, from 500 MeV/A ^{208}Pb + p measured at GSI in Ref. [61] (squares) compared with CEM03.03F results and with calculations by MCNP6 using CEM03.03.

muons: These reactions still have to be simulated with CEM, below several GeVs. In addition, INCL4.6 does not describe reactions induced by nuclei heavier than $\sim^{12}C$, and does not work at high energies, above ~ 10 GeV: Such reactions still have to be simulated in MCNP6 with LAQGSM, as no other event-generators can calculate them.

Besides the points discussed above, there are several other poor approximations and "little things" we do not like in the current version of GEM2. For these reasons, development of a new, better than GEM2, universal, based more on theory rather than on available experimental data, evaporation/fission model for our CEM and LAQGSM event-generators is necessary. Such work would require a significant amount of effort and funding, and would be probably a good subject for a PhD thesis.

What is more, while developing a new evaporation/fission model for MCNP6, it would be possible to address at the same time also the multifragmentation and fission-like binary decay problems discussed in the previous section, producing a universal de-excitation model accounting for all reaction mechanisms shown in Fig. 17.

Actually, we have proposed development of such an universal de-excitation model several times (see, e.g., Ref. [84]), but so far our sponsors have not found funding for such work. We remain optimistic and hope that such work will be funded in the future, for a real benefit to different MCNP6 applications involving evaporation/fission reactions at energies above the data-library region (i.e., above 150 MeV).

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