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CODES AND DATA FOR SPALLATION SOURCES, BENCHMARK OF NUCLEAR SPALLATION MODELS

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ABSTRACT

A Benchmark exercise of Spallation Models has been performed under the auspices of the International Atomic Energy Agency (IAEA) in order to assess the prediction capabilities of the spallation models used in high-energy transport codes and support their further development for spallation neutron source design. The selected experimental data base includes nucleon-induced production cross-sections of neutrons, light charged particles, pions, as well as residues. Seventeen different model calculations have participated to this benchmark. Necessary tools were developed using the Fortran and Perl languages to have a convenient inter-comparison of experimental data with arbitrary combinations of models calculations. Some of the final conclusions of this benchmark exercise are presented.

1. Introduction

Designing and operating a spallation neutron source requires reliable high-energy transport codes. In these codes, the elementary cross-sections and characteristics of all produced particles are either obtained from nuclear data libraries (at energies below 150 MeV and mostly for neutron-induced reactions) or calculated by nuclear-physics models.

For several decades spallation models have been developed aiming at reproducing the particle and the residue production. The reliability of each model can only be assessed via a benchmark on experimental data. If most of the time people do their own benchmark focused on a specific use of the code, more general benchmarks are needed to clearly assess the predictive capability of the available spallation models, in order to help developers and end-users.

The idea to benchmark spallation models is not new. In 1994 a first benchmark on particle (neutron and proton) production was undertaken [1]. The goal was to test the models, with two targets, ^{90}Zr and ^{208}Pb at seven incident proton energies from 25 to 1600 MeV. The method to analyze the results from the 18 model participants was based on a qualitative rating (from 1 to 3). A second benchmark was organized in 1997 focused on residue production [2]. The data used were excitation functions obtained with 5 targets (O, Al, Fe, Zr and Au) and energies from thresholds to 5 GeV. 22 models participated and another method to analyze was used, based on a statistical deviation factor (F) [2]. In both benchmarks, very large discrepancies between the model-participants were found, partly due to the fact that some models were more suited for low energy, i.e. below 200 MeV, while others were more adapted to high energy. The conclusions were that modeling calculations on a predictive basis may at best have uncertainties of the order of ± 50% for neutrons and a factor of two for residues.

Since 1997 a lot of new experimental data have been measured (neutrons, light charged particles and residues) and model developers have worked a lot to improve existing models or propose new ones. Meanwhile, new spallation-based facilities have been proposed. If some facilities already exist (ISIS, SINQ, etc.) or have been recently built (SNS and J-PARC), developments of new targets are still in progress, and the new spallation source in Europe (ESSS) or China (CSNS), for example, should use up-to-date spallation codes or at least know the quality and shortcomings of the codes they use. This is why it was decided to undertake a new spallation benchmark under the auspices of IAEA.

2. Background

A first workshop was held in Trieste in 2008 in order to organize the benchmark exercise, present the physics ingredients of the models [3] that could participate to the exercise and select the set of experimental data to be calculated by the models. For the particle production (neutrons, light charged particles from proton to alpha, and pions), the chosen observables are double differential cross sections (DDXS), but average multiplicities and multiplicity distributions have been added for neutrons. For residue production, the selected data include isotopic cross-sections, mass and charge distributions measured by the reverse kinematics method but also excitation functions. Most of the time the projectile is proton. Different targets have been considered with focus on Pb and Fe, as representatives of target and structure materials respectively, and the energy range goes from 20 to 3000 MeV.

Once collected and formatted these data were uploaded on a dedicated web site [4] as, later, the calculation results provided by the participants. The results of the 17 spallation model or model combinations are available and compared to the data. Tools (Fortran codes and Perl script) have been developed to draw all figures (around 10000) and calculate deviation factors (statistical factors, figures of merit). These factors were added to help the analysis. If the figures give all information in a qualitative way, the deviation factors quantify the information for a specific feature (mean value, shape, etc.).

A first and preliminary presentation of the calculation results by their authors was done during a satellite meeting of the AccApp'09 conference in Vienna followed by an expert meeting at IAEA in October 2009. This last meeting concluded on the way to present on the web site the figures and which deviation factors should be used.

Finally in February 2010 a second workshop devoted to the benchmark analysis was held at the CEA-Saclay. During the first part, global analyses of the results were presented and, in the second part, each model developer explained the qualities and shortcomings of its model and discussed possible improvements.

3. Analysis with emphasis on impact for spallation sources

Obviously, neutron production calculations have to be as reliable as possible when designing a neutron spallation source. However, correct predictions of light charged particles (LCP), in particular tritium and helium, and residues in the spallation target and surrounding materials are important as well, most of the time for radioprotection and safety issues. As regards residues, β/γ or α emitters, delayed neutron progenitors that can be produced in the target, in particular volatile elements in the case of liquid metals, are some examples of what must be properly estimated. In this section we present the global analysis of the benchmark in three sub-sections: neutrons, LCPs and residues, and give some particular examples of interest for spallation neutron sources.

The global analysis of the agreement between a model and the experimental data is based on a coarse eye-guided rating of all sets of data and done independently for double differential cross sections of neutrons and LCPs and for mass, charge, and isotopic residue production. R. Michel suggested the rating used for neutrons and residues, F. Gallmeier the one for LCPs (Table I).

Table I. Ratings used to analyze the benchmark results: Neutron, residues (upper part) and LCPs (lower part)

Quality	Points
Good	2
Moderately good, minor problems	1
Moderately bad, particular problems	-1
Unacceptably bad, systematically wrong	-2

Acceptance band [eval/x ; eval*x]	Points
x=5	1
x=3	2
x=2	3
x=1.4	4

Figures shown after aim at illustrating the main trends, but not at comparing one model to another, which is beyond the scope of this paper. This explains why we preferred to present more figures even if sometimes names of the models are difficult to read. The full-size figures are available on the web site [4].

3.1. Neutron production

As mentioned previously, three observables have been studied for neutrons: double differential cross section (DDXS), average multiplicity and multiplicity distribution. The rating described in the upper part of Table 1 was used for DDXS divided into four energy bins representative respectively of the evaporation, pre-equilibrium, pure cascade and quasi-elastic regions. In order to check the reliability of such a method, which may seems a priori somewhat subjective, two different people rated the calculated DDXS. The first one had in mind not only neutrons but also LCPs and residues which are known to be more difficult to reproduce while the second gave a more relative rate from +2 for the best to -2 the worst model. Then, as it can be seen below (Fig. 1), the range is larger for the second one than the first one.

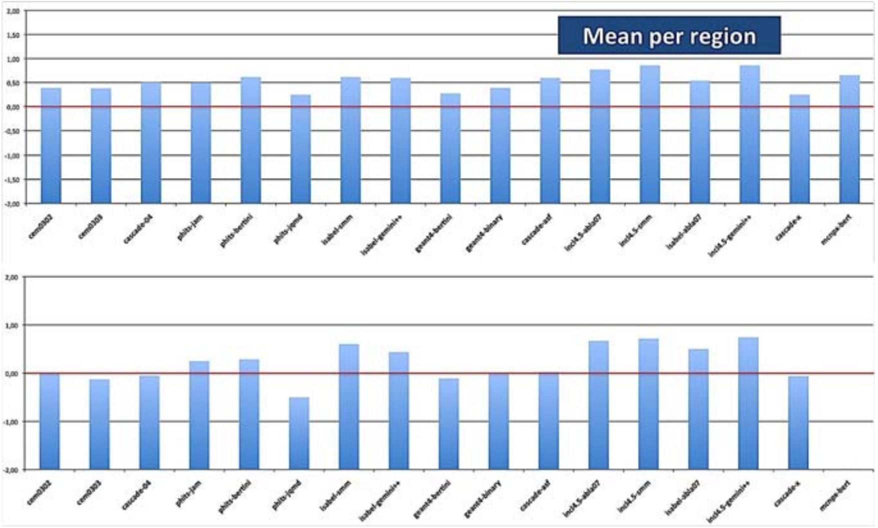

Fig. 1. Rating results obtained using the method given in the upper part of Table 1, divided by the maximum number of points, for neutron DDXS. These results were obtained by two different people.

Nevertheless the same trends are drawn, except when large statistical fluctuations on the model calculation results exist (case of PHITS-JQMD and cascade-asf (less pronounced)). Although all models can be further improved, the results are rather good and if some models are better than the others, the differences are not so strong. Definitely, it can be said that the quality of the models has been considerably improved since the 1994 benchmark.

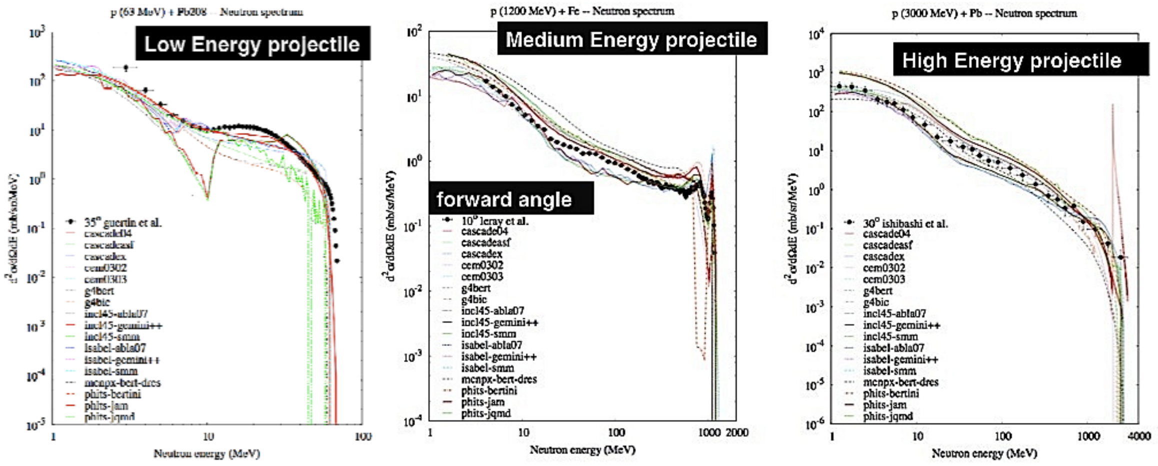

Fig. 2. Neutron spectra at particular angles for three reactions. From left to right: p(63 MeV)+Pb (35°), p(1.2 GeV)+Fe (10°) and p(3 GeV)+Pb (30°). All models are plotted.

We can divide the data sets according to the projectile energy in three regions: low (< 100 MeV), medium (~ 1 GeV) and high energy (> 2 GeV). Examples of results are displayed in Fig. 2. At low incident energies, the models have generally difficulties to fit all the details of the experimental data, which is not surprising since, at these energies, the physics hypotheses inherent to intranuclear cascade models are not valid. However, since data libraries do not exist for all nuclei between 20 and 150 MeV, models have often to be used. Therefore it is important to check their reliability and, actually, some of them are not so bad. The medium energy is generally well described by all models, but they have still some problems for high-energy neutrons on forward direction with the quasi-elastic and quasi-inelastic peaks. Finally even at 3 GeV spallation models give good results, except one model at very high energy and a set of models in the evaporation region (Fig. 2). It has to be mentioned that the region corresponding to neutron energies between 20 and 100 MeV, generally called the pre-equilibrium region, is sometimes less well reproduced, irrespective of the use of an explicit pre-equilibrium model in the calculation.

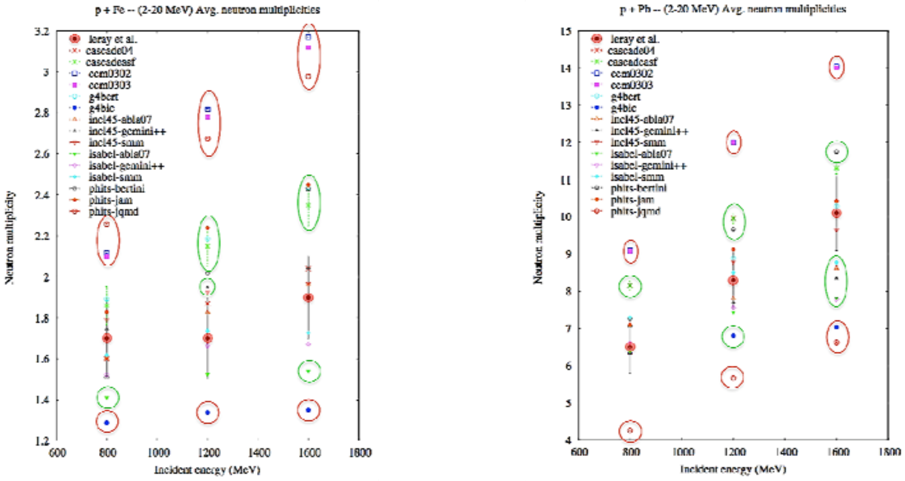

Fig. 3. Neutron average multiplicities for Iron (left) and lead (right) targets at 3 energies (0.8, 1.2 and 1.6 GeV). Here are only the low energy neutrons (below 20 MeV). All models are plotted.

Average multiplicity is an observable directly related to neutron production in spallation targets. The models have been compared for two targets (Fe and Pb) and three energies (0.8, 1.2 and 1.6 GeV). In Fig. 3 we show the results for low energy neutrons (< 20 MeV) which are the major part of the produced neutrons, but the conclusions are the same with the high-energy region (> 20 MeV). The worst case is for some models with iron, but always below a factor 2, and many models fit well the data for both high and low energy neutrons, for iron and lead. Generally lead is better reproduced, but with more models outside the error bars. Table II summarizes the reliability of our set of models.

Table II. Summary of the global average multiplicity analysis (C/E: calculation/experiment).

Reliability	Fe (< 20 MeV)	Fe (> 20 MeV)	Pb (< 20 MeV)	Pb (> 20 MeV)
50% < C/E < x2	4 models			
C/E < 50%		6 models	4 models	
C/E < 30%	6 models	3 models	8 models	2 models
Close to error bars				10 models
Within error bars	5 models	6 models	3 models	3 models

3.2. Light charged particle production

LCPs (proton, deuteron, triton, helium-3 and alpha) are abundantly produced in spallation reaction and are a concern for material damage issues. For instance, helium can be responsible of swelling in the structure materials in particular the window separating the target and the accelerator vacuum. Moreover, tritium production is often an issue from the radioprotection point of view.

The rating used is described in the lower part of Table1 and the results averaged on all models given in Table III. It is clear that LCP production is much more difficult to well describe than neutron production. Fig. 4 shows the rating for each model and for the different types of LCPs (p(1.2 GeV)+Ta). As regards composite particles, it has to be stressed that the high-energy tail observed in the experimental data cannot be reproduced by models which have not a specific mechanism to emit such particles, as coalescence in intranuclear cascade. This concerns 7 of the models and explains why proton has a better rating than the others. Fig. 4 shows this lack in the case of tritium production, but also gives hope, since at least two models describe well the whole spectrum.

Table III. Rating results obtained for light charged particle double differential cross sections.

Emitted particle	Code-Data Averaged rating	
protons	2.4	(i.e. within a factor 2-3)
deuterons	1.2	(i.e. within a factor 4)
tritons	1.2	(i.e. within a factor 4)
He-3	0.9	(i.e. within a factor 5)
alpha	1.3	(i.e. within a factor 4)

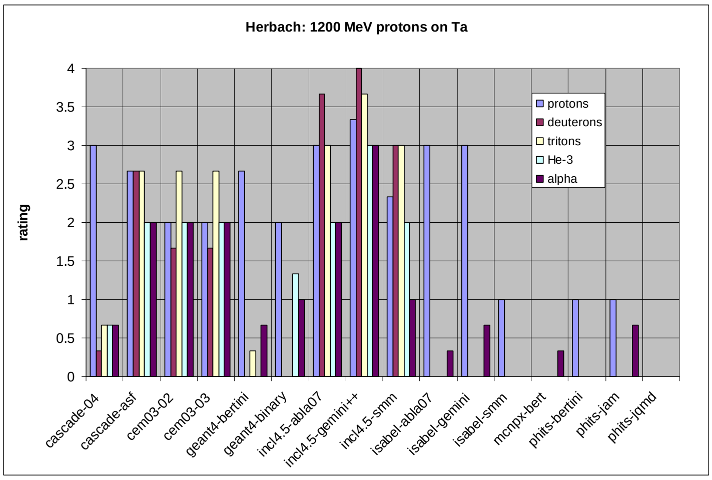

Fig. 4. Rating obtained for each model for the different types of LCPs (p(1.2 GeV)+Ta). Models having no mechanism to produce high-energy composite particles have not been rated for these type of LCPs.

3.3. Residue production

Residue production, as LCP, is more difficult to fit to the data than neutron production. We give in Fig. 5 the rating obtained for isotopic production with 3 targets (Fe, Pb and U) and 3 energies (300, 500 and 1000 MeV). It can be seen that the differences between models are really significant in this case. However, compared to the situation met in the former benchmark [2], one can state that in many reaction regimes considerable progress has been made by the modellers during the past decade. Thus, there is hope, though there is still room for improvements. Results of the crude rating for the agreement between theory and experiment for the isotope distributions are given in Fig. 5. The maximum number of available point was 28, the minimum -28. Clearly, none of the models and codes meets all the requirements, but there are significant differences demonstrating that some codes perform much better than others. There are also codes which generally perform badly and which need conceptual improvements.

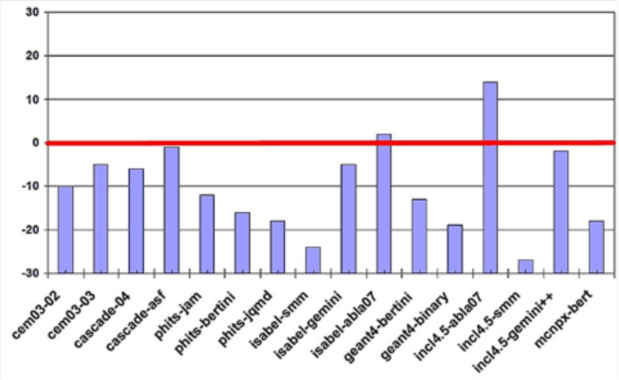

Fig. 5. Rating of the results of 16 participants for predicting the isotope distributions measured by inverse kinematics for iron, lead, and uranium at all energies.

Examples of the detailed results are given in Fig. 6. The charge distribution of residues produced in p+^{56}Fe at 1 GeV shows that a lot of models have difficulties to predict correctly intermediate mass fragments (Fig. 6 left side).

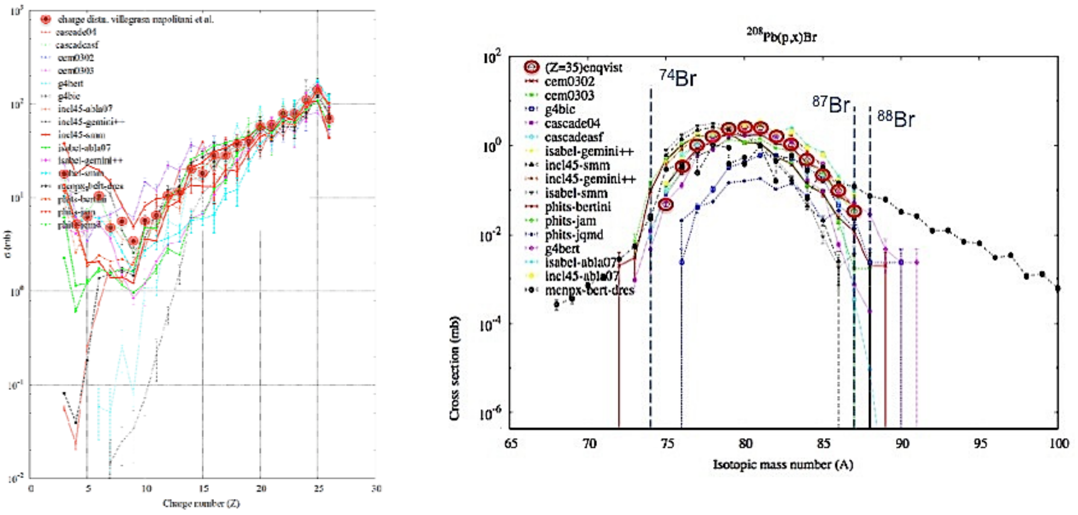

Fig. 6. Charge distribution (^{56}Fe(1 GeV.A)+^{1}H) on the left part and on the right part Br mass distribution from ^{208}Pb(1 GeV.A)+^{1}H. All models are plotted.

The isotopic distribution of bromine produced (by fission) in the p+^{208}Pb reaction at 1 GeV is displayed in Fig. 6 (right side), some isotopes being of interest for radioprotection, as the two delayed neutron precursors, ^{87}Br and ^{88}Br. This illustrates the large discrepancies between the models, both in cross-section values and in shape of the isotopic distribution.

Finally Fig. 7 shows, as an example, the difficulty to reproduce an excitation function in shape and sometimes order of magnitude for some models, but also the danger to extrapolate results from a given projectile energy to another.

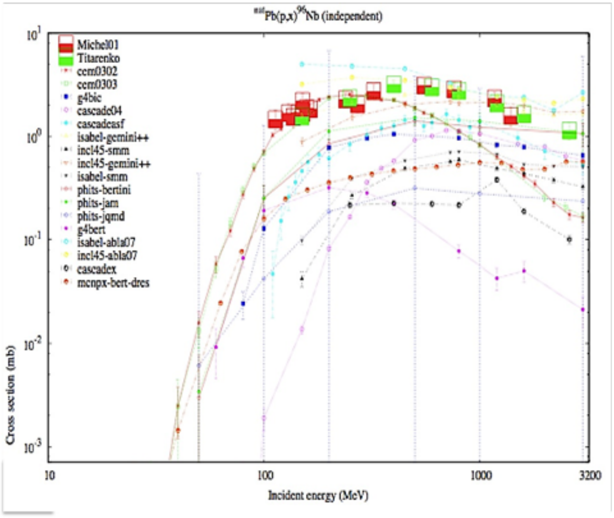

Fig. 7. Excitation function of the ^{96}Nb isotope obtained with p+Pb reaction. Data (red and green squares).

4. Conclusions

The new benchmark of spallation models, performed under the auspices of the IAEA, covers more than 40 reactions on 10 different targets induced by nucleons with energy going from 20 to 3000 MeV. Seventeen models or model combinations have participated to the exercise. Data and calculation results are available on a dedicated web site [4]. The global analysis, presented briefly is this paper, have shown that models are globally much more reliable than they were at the time of the two previous benchmarks [1, 2]. However, there is still a lot of room for improvement, in particular for the prediction of residues and composite light charged particles. If some models seem globally better than others it has to be stressed that the complexity of the spallation reactions forces to be careful with any kind of extrapolation, especially concerning projectile energy.

5. References

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