Review Paper

Benchmark of Nuclear Spallation Models

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Abstract. A summary of the satellite meeting on the Benchmark of Nuclear Spallation Models and an overview of various codes/models participated in this benchmark is presented here.

1. Introduction

Spallation reactions, and their by-products, play an important role in a wide domain of applications ranging from neutron sources for condensed matter and material studies, transmutation of nuclear waste and rare isotope production to astrophysics, simulation of detector set-ups in nuclear and particle physics experiments, and radiation protection near accelerators or in space. Understanding the importance of the spallation processes, experts from all around the world developed simulation tools and/or nuclear model codes to know the outcome, especially information about the particles and nuclei generated by these processes. Usually, the relevant simulation tools are developed on the basis of some physics processes and/or predictions, such as Monte-Carlo implementations of Intra-Nuclear Cascade models, Quantum Molecular Dynamics models, and so forth. The use of any simulation tools can only be efficient if the degree of reliability in the description of the basic physical processes is known for any given purpose. It is possible to know the predicting capabilities (strengths and weaknesses) of Spallation Models by initiating a comparative study with agreed sets of experimental data.

Early in 2008 an expert meeting (http://www-nds.iaea.org/spallations) on model codes for spallation reactions had been organized by IAEA and the Abdus Salam International Center for Theoretical Physics (ICTP). The experts had discussed in depth the physics bases and ingredients of the different spallation models and the available experimental data as well. Since it is of great importance to validate the abilities of the various codes to predict reliably the different quantities, it has been agreed to organize an international benchmark of the different models developed by different groups worldwide.

This benchmark is organized under the auspices of IAEA and an International Advisory Board was formed to analyze the results to better understand the physical basis, approximations, strengths and weaknesses of the currently used spallation models and codes. A satellite meeting on "Benchmark of Nuclear Spallation Models" was organized in association with the Accelerator Application

Conference'09 to assess the progress of the previously launched benchmark activities, to have detailed discussion among the participants and the organizers, and to define the benchmark strategy for a successful achievement of the goals. The satellite meeting was continued for two full sessions in two days. In the first session, all participants presented the assumptions, methodology, successes & failures of their codes to produce the results for the benchmark exercise. A list of the participants and their activities held in the Satellite Meeting is presented in Table 1. A concrete description of all presented codes is given in the below section.

2. Overview of the Presented Models

Table 1: Summary of the participants and their activities held in the Satellite Meeting

Participants	**Activities/presentations**
S. Leray, France	Introduction to the Benchmark of Spallation Models
J. Cugnon, Belgium	Results obtained with INCL4
Y. Yariv, Israel	ISABEL INC Model for High-Energy Hadron Nucleus Reactions
V. Ricciardi, Germany	Results of the de-excitation code ABLA07
D. Mancusi, Belgium	Comparison between the SMM and GEMINI++ de-excitation models
S. Kailas, India	Applications of Monte Carlo method in Spallation Physics
K. Gudima, Moldova	Benchmarking the CEM03.03 event generator
J. Quesada-Molina, CERN	Results obtained with nuclear models of GEANT4 in IAEA Benchmark of Spallation Models
J. Quesada-Molina, CERN	Results obtained with nuclear models of GEANT4/CHIP
N. Matsuda, Japan	Results obtained with PHITS
M. Khandaker, IAEA	Tools for Benchmarking of Spallation Models & First results

2.1. Results with INCL4

The new version INCL4.5 of the Liège intranuclear (INC) model is presented here. All the new ingredients compared to the standard version of INCL4.2 are given with some detail. They bear on the mean potentials of nucleons and pions, the included cluster production model, the Pauli blocking, the treatment of soft collisions and a somehow relaxed definition of participants. Except for the first modification, which is determined by known phenomenology, these modifications introduce some parameters which are being fixed by comparison with illustrative experimental data. The predictions for the cluster emission are much better and generally quite satisfactory with INCL4.5 in the whole range of incident energy stretching from 63 to 2500 MeV. Neutron spectra are not really changed at high energy. At low energy, the predictions of INCL4.5 are definitely better since the predictions of INCL4.3 were renormalized on the experimental reaction cross sections. Concerning the shape of the neutron spectra, the results of INCL4.5 are only and not always slightly better, though not sufficient. The shapes of the proton spectra are not very much changed either. However, they have the tendency to be underestimated (in the cascade stage). Pion production is somehow improved with INCL4.5.

Concerning residue production, the deep spallation side of charge and mass spectra, is significantly improved with INCL4.5 in p+Fe and p+Pb processes. In p+U, the improvement leads even to some overestimation. In p+Fe, the yield is still too low for the very low mass side. Concerning the isotropic distributions, if there is a slight improvement in INCL4.5, the shape of the distributions for residues of charge close to the target charge are only slightly affected and the discrepancy mentioned in the introduction persists.

It is hard to trace back the effects of one of the modifications introduced in INCL4.5 and to associate them with the improvement of one or the other of the predictions. Of course, it is clear that the modification of the cluster emission module is responsible for the improvement of the cluster production cross sections, especially at low energy. Similarly, the new treatment of soft collisions is responsible for better predictions of the particle spectra at low energy. Though not clear enough, the modifications of the average potentials for nucleons and pions have contributed to the improvement of the pion production cross sections. The effect of the other modifications is too largely intermingled with those of the de-excitation models to draw any definite conclusion. It should be remarked that sometimes the modifications have a negative effect. For instance, the proton spectra are less good with the introduction of the cluster production module. Finally, INCL4.5 offers a clear and substantial improvement of the standard INCL4.2 version. The most noticeable case is the isotopic distributions for isotopes close to the target, which are still overestimated on the neutron rich side. Further work is still needed to obtain a model for an adequate predictive power for ADS applications.

2.2. ISABEL INC Model for High-Energy Hadron-Nucleus Reactions

ISABEL is a "time like basis" Monte Carlo realization of an INC model for hadron-nucleus and nucleus-nucleus collisions. It is a direct descendant of the original implementations of Serber's model [R. Serber, Phys. Rev. 72, 1114 (1947)] and a generalization of the VEGAS [K.Chen et al., Phys. Rev. 166, 949 (1969)] and ISOBAR [G. Harp et al., Phys. Rev. C10, 2387 (1974)] INC codes. The general idea of Serber is to follow the energetic projectile as it classically scatters in the target. On its way it excites particles pulling them out of the Fermi sea. Those particle either leave the target volume, or if they are not energetic enough contribute to the residual excitation of the target, to be de-excited by some evaporation (or pre-equilibrium process).

INC models reproduce successfully wide variety of experimental data of hadron and pion induced reactions, using a small number of adjustable parameters, most with clear physical meaning. The main purpose of the INC models is to fill the high-energy gap in existing experimental cross-section libraries, which are limited to incident energies of 150 MeV or even, for some isotopes, 20 MeV. For calculations of residues, there is a need to use models already above 20MeV. The INC models treat the interaction of incoming projectile with the nucleus as a series of independent collisions using on-mass-shell free particle-nucleon cross sections. The colliding particles are treated as classical point-like objects moving between collisions on well defined trajectories in the target potential well. The collision processes are treated as classical, energy and momentum conserving, scatterings. Collisions violating the Pauli Principle are not allowed – this is the single significant “quantum” property of the models.

High energy cluster (α, d, He-3…) production is out of the scope of INC models. In order to calculate those “extra prescriptions” are used. In the “coalescence” model the vicinity (configuration, momentum or phase space) of escaping particle is searched for potential particles to share its energy and form a cluster. An alternative “kick-out” process assumes existence of “virtual” clusters in the nucleus which elastically scatter with the cascading particles and then, taking into account their survival probability, escape the nucleus. As in ISOBAR, pion production and absorption modes are included in ISABEL via pion-nucleon isobar formation in nucleon-nucleon scattering, therefore no additional modes of pion production or capture are included. ISABEL was used without the additional coalescence model; no attempt was made to predict the production of high-energy “heavy” fragments.

The presentation in this meeting reflects that ISABEL INC model seems to be able to produce accurate results on many observables, such as cross sections for emission of neutrons, protons, composite particles, pions, residues and so on.

2.3. *Results obtained with ABLA07*

The de-excitation code ABLA has been continuously developed in the last years, guided by the empirical knowledge gained in a campaign of spallation and fragmentation experiments performed at GSI, Darmstadt. The better insight into the reaction mechanisms lead to a highly improved version of the code, namely ABLA07,

which is a dynamical code that describes the de-excitation of the thermalised system by simultaneous break-up, particle emission and fission. Simultaneous break-up is considered as the cracking of the hot nucleus into several fragments due to thermal instabilities. The description of particle evaporation is based on the Weißkopf-Ewing formalism [V.F. Weisskopf and D.H. Ewing, Phys. Rev. 57 (1940) 472], while the fission decay width is calculated taking into account dynamical effects [B. Jurado et al., Phys. Rev. B 533 (2003) 186]. The physical content and technical algorithms of this code are described in great detail in the authors' contribution to the proceedings of the “Joint ICTP-IAEA Advanced Workshop on Model Codes for Spallation Reactions„ held in Trieste, Italy, 4-8 January 2008.

In this work the de-excitation code ABLA07 was coupled to three different models of the collision stage: INCL4, ISABEL, and BURST. The spallation at 1 GeV of three systems is analyzed: 56Fe, 208Pb, and 238U. The discrepancies among the different variables (yield, average atomic number, excitation energy, and angular momentum), which characterize the remnants predicted by the three models, amount in most cases to about a factor of 2. The following de-excitation process does not wash out these differences. This indicates that adapting a de-excitation model to a given INC model, such to provide the best final results when combined together, does not automatically assure high predictive power in regions not tested before. Larger cross checks and benchmark with many experimental data are therefore needed to fix the various models.

2.4. *Comparison between the SMM and GEMINI++ de-Excitation Models*

Nuclear de-excitation codes can be coupled to intra-nuclear cascade models to provide coherent and comprehensive descriptions of spallation reactions above ~ 150 MeV. The INCL4.5 cascade code has been coupled with the SMM and GEMINI++ de-excitation models and simulations of proton-induced spallation reactions have been performed. The results presented represent a subset of the simulations that have been performed for this Benchmark of Spallation Models.

The INCL4.5/GEMINI++ model seems to be able to produce accurate results on many observables, such as residue yields, and cross sections for emission of neutrons and composites (alpha particles). This good accuracy, however, comes at the price of a high computational cost. The INCL4.5/SMM code does not suffer from the heavy computational penalty of GEMINI++, but its results are generally less accurate. Three main reasons were identified for these shortcomings. Firstly, the evaporation/fission module of SMM is quite simple; one could probably ameliorate some of SMM’s predictions by refining some of the ingredients, such as level densities, Coulomb barriers, or may be by choosing other evaporation/fission formalisms. Secondly, the free parameters of SMM have not been adjusted to the INCL4.5 remnants; it is thus conceivable that the agreement could be improved with some fine tuning. Thirdly, many of the SMM results reproduce for this benchmark would be improved by the adoption of a pre-equilibrium stage between cascade and de-excitation.

2.5. Applications of Monte Carlo method in Spallation Physics

The CASCADE code realize the particle transport by different stages: 1) sampling of particle (ion) mean free path in the medium taking into account the energy loss of a charged particle and a possible decay of non stable particles (π0, π+, π-). All π0 mesons are considered to decay into γ-quanta at the point of their creation. The ionization losses of pions, protons, and light ions are calculated by Sternheimer's method [R. Sternheimer, Phys. Rev. 145, 247 (1966)]. In the lower energy region Lindhard's approach [L. Lindered et al., Kon. Den. Vidensk. Selsk. Nat.-Fys. Medd. 33, 14 (1963)] is used, and a semi-phenomenological procedure is applied for the heavy ions. 2) Simulation of the particle/nucleus interaction with a nucleus was considered along its path. In case of inelastic interaction the CASCADE code considers three stages of reaction for calculations. a) intra-nuclear cascade: In this part of the calculation, primary particles can be re-scattered and they may produce secondary particles several times prior to absorption or escape from the target. Cross-sections of the hadron-nucleus collisions are calculated based on the compilations of the experimental data. To calculate nucleus-nucleus cross sections analytical approximations with parameter defined in ref. [V. Barashenkov and H. Kumawat, Kerntechnik 68, 259 (2003)] were used. Criteria of transitions from intra-nuclear cascade to pre-equilibrium stage are the cutoff energy, below which the particles are considered to be absorbed by the nucleus. b) pre-equilibrium stage: In this part of the reaction, relaxation of the nuclear excitation is treated according to the exciton model of the pre-equilibrium decay. The relaxation is calculated by the method based on the Blann's model [S. Mashnik and V. Toneev, JINR p4-9417, Dubna, 1974]. Proton, neutron, deuteron, tritium, He3, and He4 are considered as the emitted particles in the pre-equilibrium and the subsequent equilibrium stage. Transitions from pre-equilibrium to equilibrium state of the reaction occurs when the probability of nuclear transitions changing the number of excitons n with $\Delta n = +2$ becomes equal to the probability of transitions in the opposite directions with $\Delta n = -2$, c) equilibrium stage: This part considers the particle evaporation/fission of the thermally equilibrated nucleus. The code uses 26-group constants for neutron transport cross-sections below 10.5 MeV. The neutrons can moderate by numerous elastic collisions; can make fission in case of fissile/fertile materials and finally captured in (n, γ) reaction. It was assumed that cascade particle is stopped if its energy is less than the boundary energy Eb which equals to 2 MeV for pions, proton and deuteron, 10 MeV for tritium, and 10 MeV/nucleon for all heavier nuclei.

However, in this intercomparison the CASCADE-04 code reproduces well the experimental data for neutron and proton emission, but shows deviation of factor 2 or more for the composite particles. A general observation for residue production is that the theoretical values are in good agreement with the experimental data close to the target mass number as well as at the peak of the isotopic distribution but the disagreement increases at the tail of the distribution. The widths of the calculated distributions are less compared to the experimental data almost in all cases. It is to be noticed that even-odd effect is still seen in the calculations which are absent in the experimental data. The pairing correction is included in the calculation which reduces the effect but does not vanish completely. The big spallation region that comes after a long chain of the multi-step direct and evaporation mechanism, is underestimated by the present version of the code. It is to be noted that these calculation are shown for the case where particle emission up to alpha are considered.

2.6. Complex particle production by CEM03.03

The INC of CEM03.03 is based on the "standard" (non-time dependent) version of the Dubna cascade model (V.S. Barashenkov, K.K. Gudima, and V.D. Toneev, JINR Communications p2-4065 and p2-4066, Dubna (1968); P2-4661, Dubna (1969); Acta Physica Polinica 36(1969) 415), improved and developed further at LANL during recent years (S. G. Mashnik et al., J. Nucl. and Radiochem. Sci. 6, (2005) A1). The coalescence, pre-equilibrium, evaporation, fission, and Fermi breakup models used by the last versions of the Cascade-Exciton Model event generator CEM03.03 have been extended recently to improve description of complex particles production from nuclear reactions. The CEM03.03 code calculates nuclear reactions induced by nucleons, pions, and photons. It assumes that reactions occur generally in three stages: the Intra-nuclear Cascade (INC) stage, the pre-equilibrium stage, and the equilibrium evaporation/fission stage. CEM03.03 uses the coalescence model to "create" high energy d, t, 3He, and 4He by final-state interactions among emitted cascade nucleons. However, if the residual nuclei after INC have mass numbers with A≤12, CEM03.03 uses the Fermi breakup model to calculate their further disintegration instead of using the pre-equilibrium and evaporation models.

Here, it has been tested on how CEM03.03 describes complex particle spectra and yields from all reactions included in the Mandatory List of this Benchmark exercise. On the whole, CEM03.03 describes reasonably well many measured data on production of d, t, He3, and He4 from various reactions. However, several problems were identified to be solved for a better description of complex particles emission from some reactions, and observed a necessity to extend the pre-equilibrium emission for fragments heavier than He4, currently neglected by CEM03.03. CEM03.03 versions describe the production of composite particles (d, t, 3He, and 4He) from nuclear reactions in a wide range of incident energies of interest to Spallation Applications better than earlier versions. As a rule, CEM03.03 describe such reactions not worse than other codes presently available, and are often much faster, which is very important in complex simulations.

2.7. Results obtained with nuclear models of GEANT4/CHIP

Geant4 is the C++, object oriented successor of Geant3. It was designed primarily to handle the problems for high energy physics, but currently is using in medical and space applications as well. It is a toolkit that provides large degrees of functionality and flexibility, many different codes including alternatives for the same regions of applicability. All major physics processes such as electromagnetic, hadronic, decay, photo- and electro-nuclear are covered by these codes. As an example, the hadronic processes include elastic, inelastic, capture at rest, neutron capture, neutron-induced fission, lepton-nuclear, and gamma-nuclear processes. Each of the processes is implemented by one or more models (which contain the physics algorithm) and cross sections (which determine the mean free path etc.).

Geant4 participated in the IAEA hadronic Spallation benchmark by submitting predictions from three hadronic models: Bertini, Binary Cascade and CHIPS. The intra-nuclear cascade models reproduce the spallation data fairly well in most cases, with Bertini performing better under some circumstances and Binary Cascade performing better under other circumstances. Isotope production with inverse kinematics can be simulated by all three models. Some obvious problems exist in reproducing the minima for the U + H reaction, but the qualitative features are reproduced. Some complications exist for light ion production from various targets. In Bertini and Binary, these problems are due to the lack of clusterization within the target nucleus as well as the absence of coalescence methods. However, the Geant4 group expect from this intercomparison that specific are will be indicated where improvement is needed. It was also mentioned in the meeting that the Geant4 group recently made an improvements to precompound processes, plan to add coalescence models for cascade stage in their models.

2.8. Results obtained with PHITS

In the particle and heavy ion transport code system PHITS, three simulation codes JAM, Bertini, and JQMD were used to describe the intermediate and high energy nuclear reactions. JAM is a simulation code based on INC (intra-nuclear cascade) model, which explicitly treats all established hadronic states including resonances with explicit spin and isospin as well as their anti-particles. Parametrization were done for all hadron-hadron cross sections based on the resonance model and string model by fitting the available experimental data. Bertini is a simulation code based on Monte Carlo calculations on intra-nuclear cascade [H.W. Bertini, ORNL-3833, Oak Ridge National Laboratory (1963)]. JQMD is a simulation code based on the molecular dynamics. A typical feature of

QMD compared with that of the INC model is that QMD can describe not only nucleon-nucleus reactions but also nucleus-nucleus reactions in the same framework. The JQMD code has been widely used to analyze various aspects of heavy ion reactions as well as of nucleon induced reactions, and has shed light on several exciting topics in heavy ion physics, for example, the multifragmentation, the flow of the nuclear matter, and the energetic particle production.

The simulation codes (JAM, Bertini, and JQMD) used here for this intercomparison describes the intermediate and high energy nuclear reactions in the particle and heavy ion transport code system-PHITS. By using these nuclear reaction models, PHITS can simulate various phenomena including hadron-nucleus reactions with energies up to 200 GeV, nucleus-nucleus collisions from 10 MeV/u up to 100 GeV/u and transports of heavy-ions in the materials as well as the neutrons down to 10-5 eV and leptons. These codes reproduce the experimental data for neutron production with a general good agreement but for proton and pion production shows deviation within a factor of two or higher. In case of neutron multiplicity, the calculations tend to be smaller than the experimental value for >20 MeV, but larger in the range of 2-20 MeV. The prediction of composite particle production is not included in the correct way in the current version of this codes or improvement is required. Concerning the residue production and also the excitation function, the codes describe well the experimental data for this intercomparison. Almost calculations agreed with the experimental data by all the mentioned PHITS-codes, but quite distorted results showed for d, t, 3He and a emissions. However, repeated calculations are in progress to provide an improved set of results for the IAEA benchmarking.

3. Conclusions and Recommendations

Necessary tools were developed to perform the benchmark activities, and presented in this meeting. Additionally, the overall status of the benchmark activities was presented as well. Some critical points to handle the benchmark data were pointed out and the possible solutions of them discussed. The first results with preliminary conclusions were shown. Later, a round table discussion was held among the organizers and all the participants of this benchmark exercise to have the clear concept of the next activities, and also fixed up the time-frame for the whole benchmark activities. However, the organizers were agreed to postponed the deadline (31th of July) to allow participants to give more results/calculations, especially for the codes which are slow and/or took more time (such as, QMD calculations) to calculate the full set of requested data. As the 2nd step of this benchmark exercise, the organizer had decided to do the statistical analysis (such as, find out the deviation factors, chi-square values and parameters, ratios of experiment to calculated values and so on), to find the indicators for the smooth and advanced ways of treating the results. An overall table/chart will be prepared by the calculated indicators for all corresponding experimental and calculated data by September 2009. In the beginning of October 2009, an expert meeting will be organized at the IAEA to find out and/or extract a real outcome from the prepared benchmark results (comparative figures, statistical data table etc.). As a consequence of the meeting, a preliminary report will be prepared for the whole benchmark activities by November 2009. Additionally, the physics analysis of this benchmark will be done by February 2010, and will be presented on the jointly organized workshop by IAEA-France (the exact place of the workshop not decided yet). However, the final outcome of this benchmark will be presented in the Nuclear Data conference in May 2010.

All information on the Benchmark activities has been posted on the dedicated website:

http://www-nds.iaea.org/spallations