Benchmark of Spallation Models (IAEA)

Analysis of neutron productions

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A typical neutron spectrum is shown below for p(1600 MeV) + Fe [xxx].

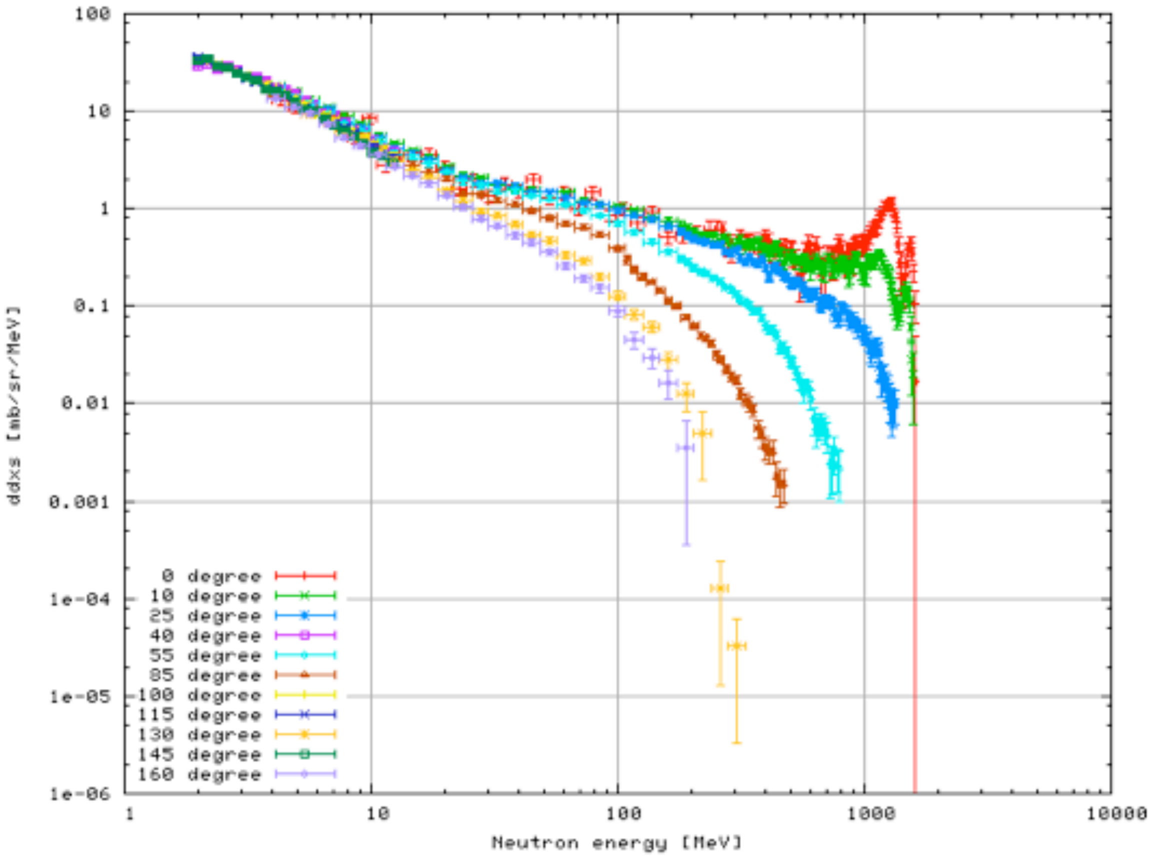


Fig. 1: Neutron spectra obtained from the reaction p(1600MeV)+Fe [xxx]

It can be divided in three energy regions: low energies, i.e. below around 20 MeV, intermediate energies, between 20 and 150 MeV and high energies above 150 MeV.
The low energy neutrons come from the evaporation phase and are isotropically emitted. Around 20 MeV slight differences with angles can appear due to a minor contribution from the intermediate energy part. The intermediate energy region is clearly anisotropic and focused in forward direction and the origin of neutrons in this energy region is either the intra-nuclear cascade or a preequilibrium stage. This last point will be address latter. The anisotropic behaviour is stronger for the high-energy part with two peaks at very forward angle: the quasi-elastic peak which is narrow and at very high energy (due to the elastic reaction between beam and nucleons in the target) and the quasi-inelastic peak at lower energy which is broader (due to the width of the Δ

resonance). The energy limits given here has been chosen to simplify the analysis and the discussion. They must not be considered as sharp values.

In the next sections we will present the main results obtained by the models that participated to the benchmark. A link between successes/deficiencies and the physics ingredients will be done when possible or at least mention as a question for the model developers.

1) Low energy - E_n < 20 MeV

Low energy neutrons are most of the times well reproduced by all models (Fig. 2). A factor 2 with the data can be observed in some cases, but usually calculations are much better and the difference between experiment and simulation is around 20-30%. The shape is good also, with maybe a slight underestimation at very low energy (~1 MeV) and overestimation at higher energy. However above 10 MeV neutrons come from evaporation but also from intra-nuclear cascade or preequilibrium that makes less important the evaporation process in this energy region. At very low energy we can see that model results are more spread out. A possible reason is the difficulty to choose the right inverse cross in the modelling of the evaporation of very low energy neutrons. These cross sections come from experimental or evaluated data, but in both cases with ground-state nuclei, which has no consequence for high-energy neutrons, but not for neutron below and around 1 MeV.
The strange behaviour of cascadex below 4 MeV is plausibly a mistake in the simulation.

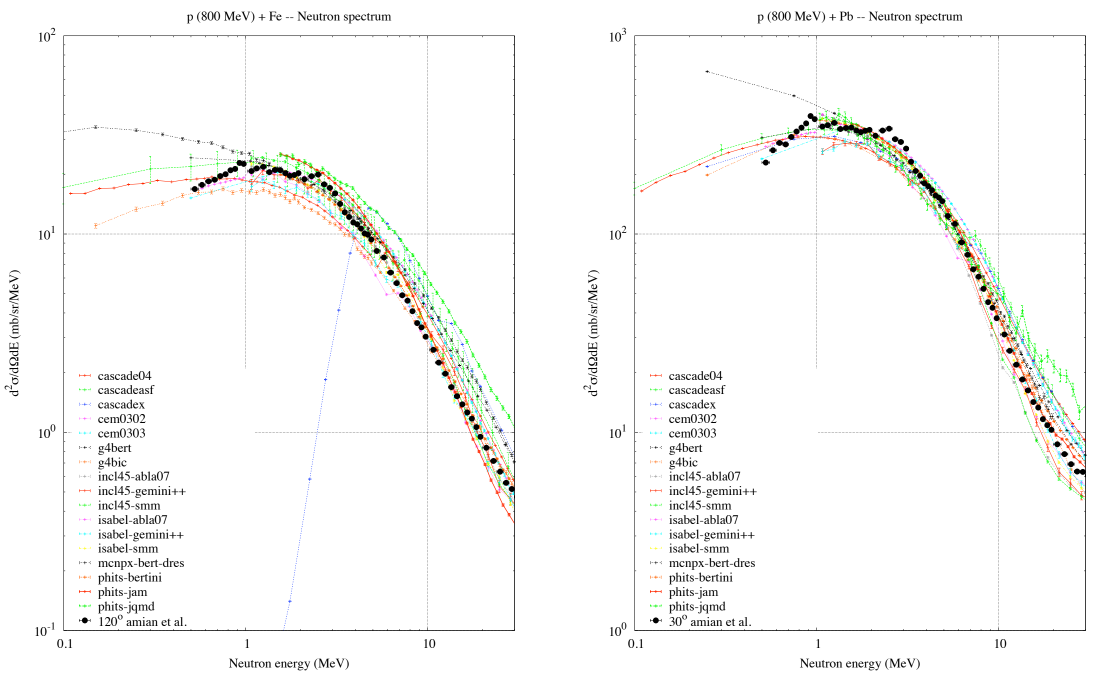


Fig. 2: Neutron spectra obtained from the reactions p(800MeV)+Fe on the left (Θ=120°) and p(800MeV)+Pb on the right (Θ=30°) [xxx]

With Fig. 3 the spread of the results is studied according the projectile energy. It has to be mentioned first that these data from SATURNE have been obtained with thick targets

(2 or 3 cm thick). This leads to an overestimation of the low energy neutron (< ~4MeV) compared to a thin target (Amian data - see Fig. 2) and has been studied and explained in [xxx].

Here again the results are good and whatever the projectile energy is. However some differences exist between the models used. These differences are much important when the projectile energy increases and for the highest energy neutron. This can probably be explained by the excitation energy of the nuclei that increases with the projectile energy. Moreover this effect is washed out during the evaporation process and so more important for high-energy neutron, i.e. at the beginning of the deexcitation.

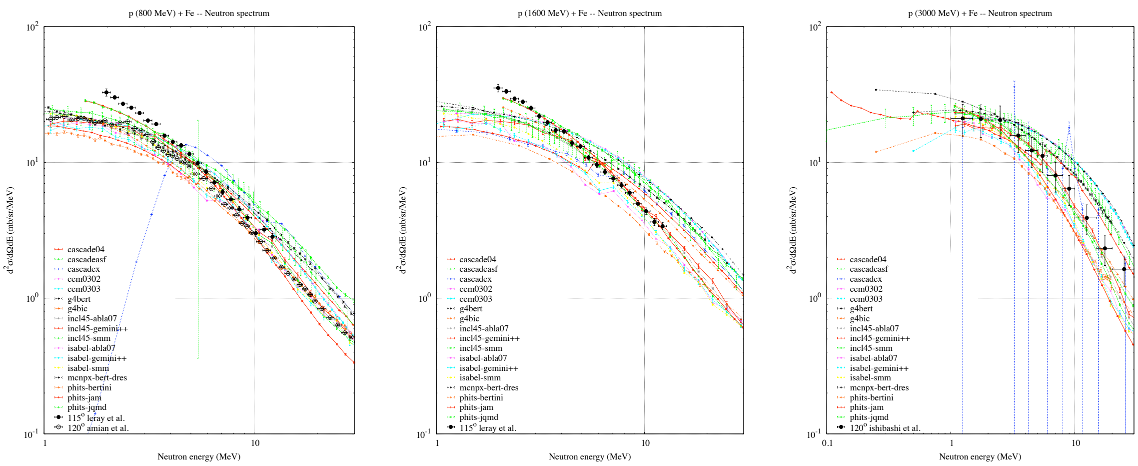


Fig. 3: Neutron spectra obtained from the reactions p(800MeV)+Fe on the left (Θ=120° [xxx] and Θ=115° [xxx]), p(1600MeV)+Fe in the middle (Θ=115°) [xxx] and p(3000MeV)+Fe on the right (Θ=120°) [xxx]

If in Fig. 3 iron was used as target, the next Figures deal with lead targets. With Fig. 4 we understand that the behaviour is the same as with iron. For a given projectile energy the spread is a little bit less pronounced with lead. That is probably because a same excitation energy leads to a smaller temperature in a heavier nucleus, then on the one hand smaller the temperature is less numerous the deexcitation channels are, and so neutron emission is favoured, and on the other hand the energy range of the emitted neutrons is smaller (Maxwellian distribution based on temperature). The importance of the intra-nuclear cascade (and preequilibrium phase for some models) in the evaporation stage seems clear with Fig. 3. The three deexcitation models used with Isabel or INCL4.5 give similar results.

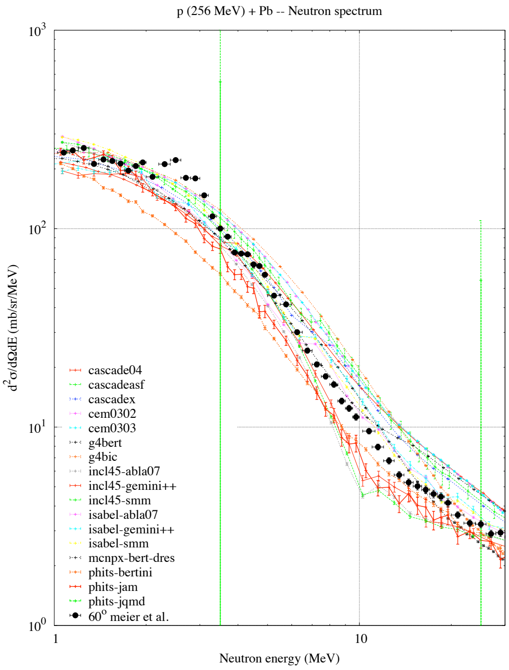


Fig. 4: Neutron spectrum obtained from the reaction p(256MeV)+Pb (Θ=60° [xxx]

For rather low energy projectile the same conclusion can be drawn (Fig. 4), except that the crossing between evaporation and intra-nuclear cascade or preequilibrium seems to be around 12 MeV for 256 MeV protons on a lead target.

This crossing is of course at lower energy if the projectile energy is below 100 MeV, as in Fig. 5 (9-10 MeV) with 63 MeV protons on lead. Spallation models should not be used for such so low projectile energies, since the intra-nuclear cascade hypothesis are no more valid: The nucleus can be no more seen as a bag of free nucleons by the projectile. Nevertheless when a transport code deals with nuclear reactions, it uses either libraries or models. However up to now libraries don't contain all needed information for reaction induced by nucleons or light cluster (up to alpha) with an energy below 150 MeV, which is more or less the low energy limit where the spallation models can be reasonably used. So transport codes use spallation models and then it is interesting to know their behaviours outside their domain of validity.
Fig. 5 shows that the low energy part, below 9 MeV, of the neutron spectrum is not so bad and the results surprisingly good. This is however not true for INCL4.5 around 10 MeV whatever the deexcitation model used. This spurious behaviour comes from a specific ingredient in the intra-nuclear cascade modelling and should be fixed.

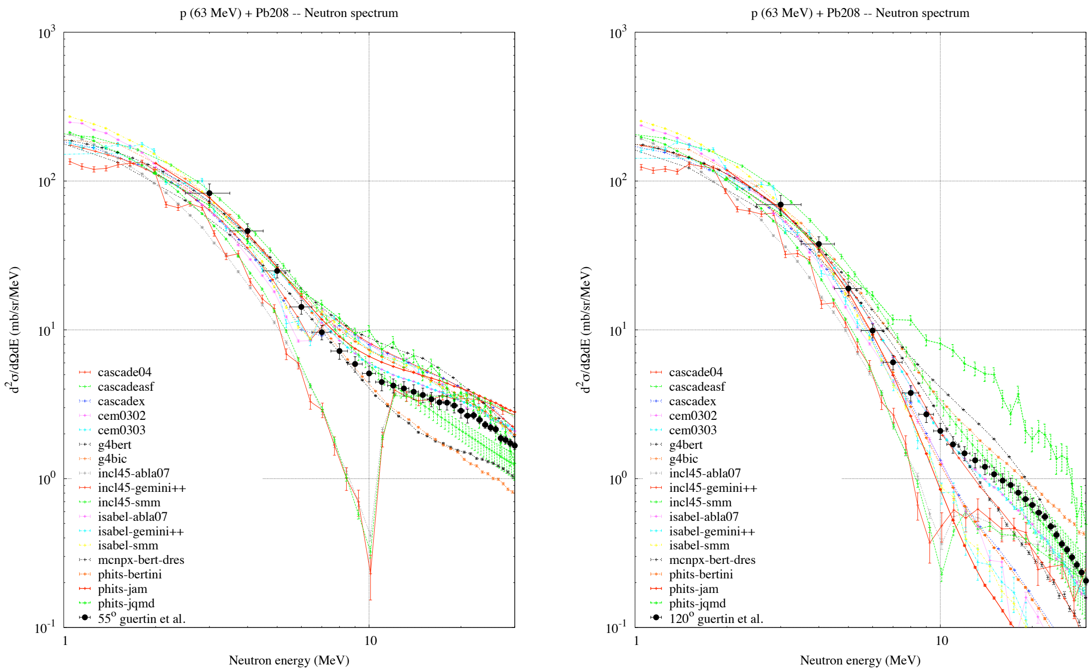


Fig. 5: Neutron spectra obtained from the reactions p(63MeV)+Pb at Θ=55° on the left and Θ=120° on the right [xxx]

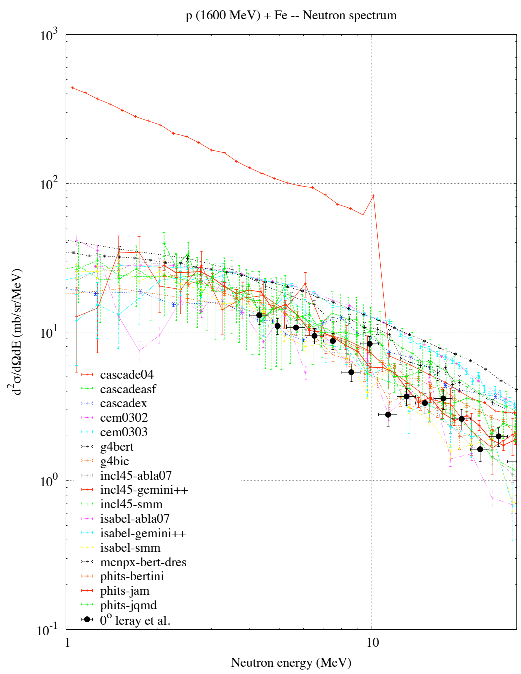


Fig. 6: Neutron spectrum obtained from the reactions p(1600MeV)+Fe at Θ=0° [xxx]

Another strange behaviour appears with cascade04 in Fig. 6. Below 11-12 MeV cross sections are multiplied by a factor 10. Simulation at 0° is always very difficult because to get good statistics with the same experimental conditions the number of run will be huge. Then, for instance, calculations are performed not exactly with the right angular aperture. Nevertheless this can't explain this jump.

2) Intermediate energy - 20 < E_n < 150 MeV

This energy region is linked to the end of the cascade or to the preequilibrium stage.

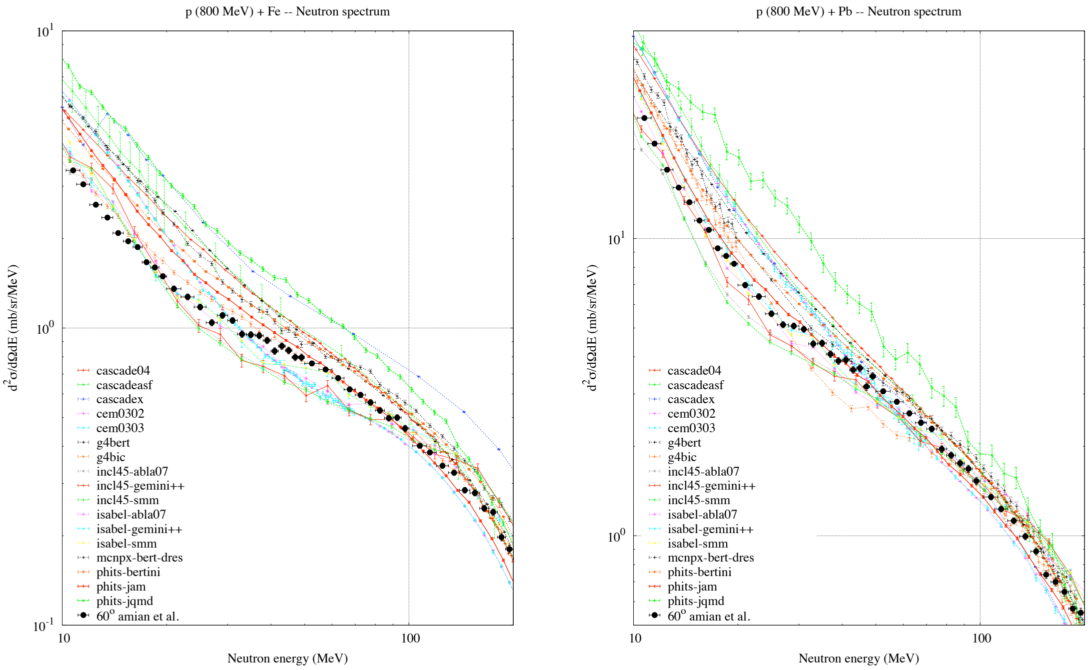


Fig. 7: Neutron spectra obtained from the reactions p(800MeV)+Fe at Θ=60° [xxx] on the left and p(800MeV)+Pb at Θ=60° on the right [xxx]

Fig. 7 shows that the shape of the spectra are quite well reproduced and simulations fit the experimental data within a factor 2 and very often within ~20%. In this case phits-jqmd clearly overestimates the data compared to the other models. However with a higher projectile energy, Fig. 8, we see that models can be lumped into two groups. The first one fits the data with sometimes a slight overestimation and the second one underestimates the data. An interesting point is that all models in the first group include an intermediate stage between intra-nuclear cascade and deexcitation, the preequilibrium phase, which is not the case for the models in the second group. This could explain the results, but unfortunately the need of preequilibrium is not so clear. For energies below this energy region, i.e. around 10-15 MeV, the "underestimate group" fits the data whereas models with preequilibrium overestimate them. This effects can also be seen in Fig. 3 with p(3000MeV)+Fe.

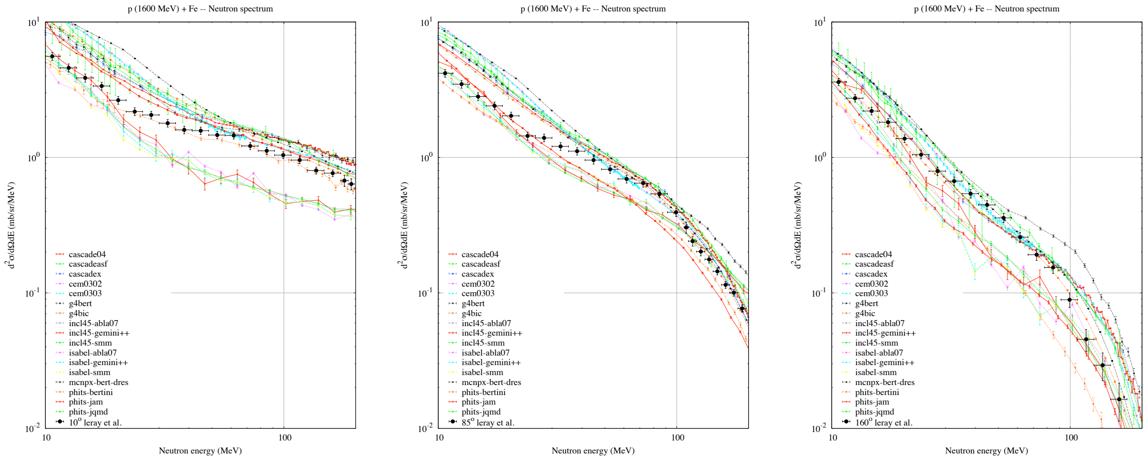
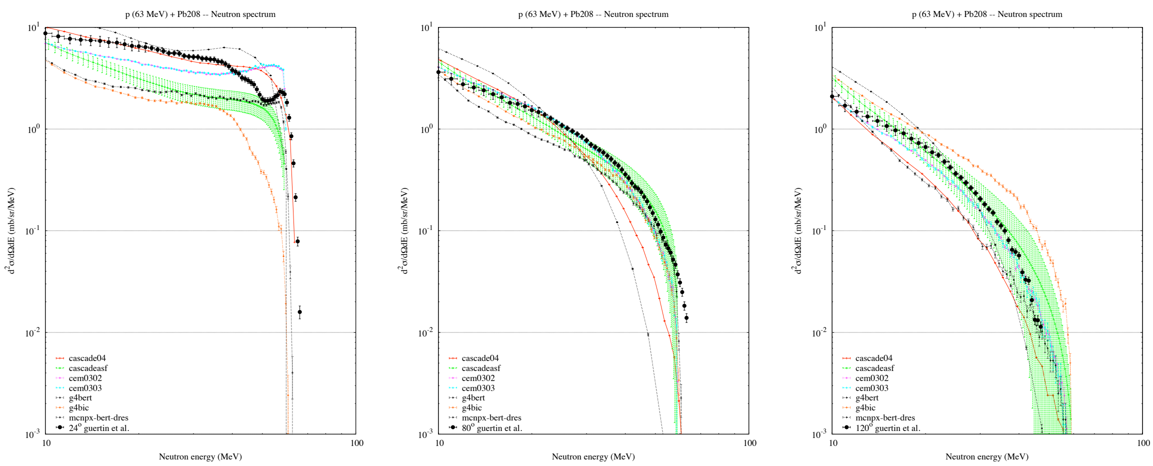


Fig. 8: Neutron spectra obtained from the reaction p(1600MeV)+Fe at three angles (Θ=10°, 85° and 160° from the left to the right) [xxx]

As already mentioned spallation models should not be used to describe low energy reactions. Nevertheless the p(63MeV)+^{208}Pb is interesting since the preequilibrium phase could play a major role in this case. In Fig. 9 we plot on the upper part models with preequilibium and on the lower part models without preequilibrium. The first group gives much better results for backward angles, while for the forward angle second group would be preferred. The situation for the intermediate angle is not so clear. In the first group some models provide very good results and in the other group phits-jqmd and INCL4.5 over- or under-estimate the data for the low energy region, whereas they are very good for the high-energy neutrons. In the case of the intra-nuclear model INCL4.5, it would be interesting to see the spectra, if the strong and spurious depression around 10 MeV could be fixed, and to see if without preequilibrium it is possible to get the same good results as the both CEM, for example.



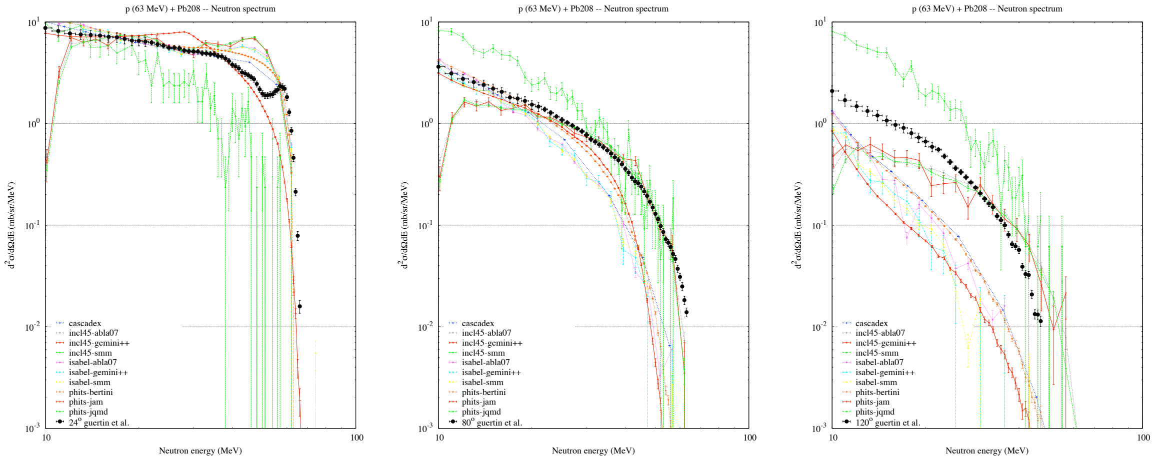


Fig.9: Neutron spectra obtained from the reaction p(63MeV)+^{208}Pb at three angles (Θ=24°, 80° and 120° from the left to the right) [xxx]. Here we split the models in two groups: with preequilibrium on the upper part and without preequilibrium on the lower part.

3) High energy - E_n > 150 MeV

Neutron emission is very anisotropic in this energy region. Then we divide the analysis in three angular domains: forward directions (Θ<45°), transversal directions (45°<Θ<135°) and backward directions (Θ>135°).

3.1) Forward angles

The main characteristic in this energy region and angular domain is the structure at very high energy (Fig. 10): Two peaks at 0° which vanish when the angle increase. The elastic peak, i.e. neutrons emitted from an elastic collision with the projectile, is narrow and around the energy beam. The second peak, called inelastic peak, come from the delta resonance. This explains why it is much larger (resonance width) and at lower energy.

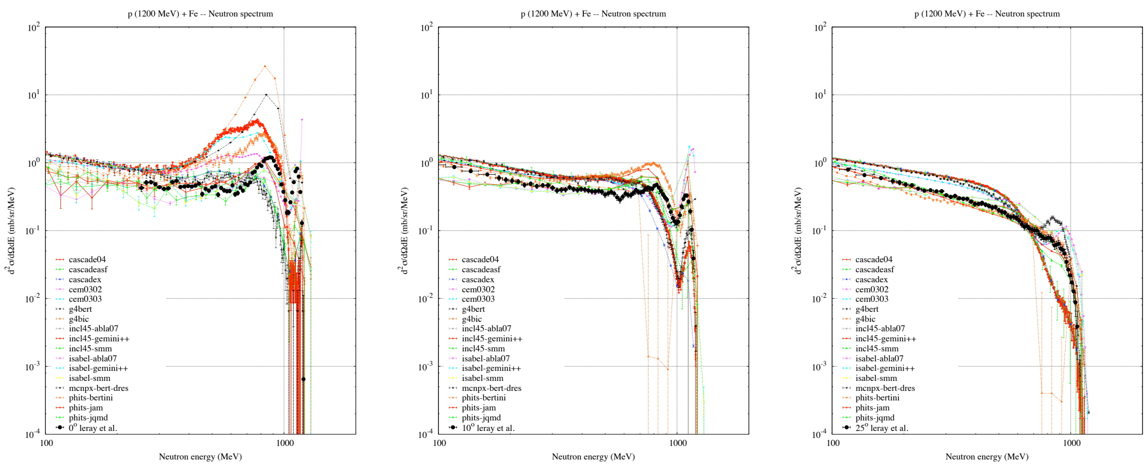


Fig. 10: Neutron spectra obtained from the reaction p(1200MeV)+Fe at three angles (Θ=0°, 10° and 25° from the left to the right) [xxx].

At 0°, as mentioned before, these peaks are difficult to reproduce (Fig. 10) because the experimental condition are not easy to simulate (compromise between angular aperture and running time). This problem disappears at 10°. The elastic peak is rather well reproduced by all models, especially the place. The height is the major problem. Some models have a too high peak like isabel, cem (factor 3 or 4), phits-jam (factor 2), some others a too low peak like geant4-bertini and cascade04. If some models have almost the right height, like geant4-bic and phits-jqmd, some others give unfortunately not enough points in this region to know exactly the behaviour (see INCL4.5 or mcnpx-bert-dres). It seems that this elastic peak still exists at 25° for some models (cem, isabel, geant4-bert) whereas it is not the case in the experimental data. In opposite the 3 "cascade" models (cascade04, cascadeasf and cascadex) miss strongly the high-energy neutrons at 25°.
The difference between the models concerning the inelastic peak is more important. Around 0° the simulation difficulty has been mentioned, nevertheless two models give a very high peak (MCNPX-bert-dres and phits-bertini), four models overestimate and are too large (both CEM, geant4-bic and casacde04) and three seems to have no peak (cascadex, cascadeasf and geant4-bertini). The other models reproduce reasonably well the shape and height.

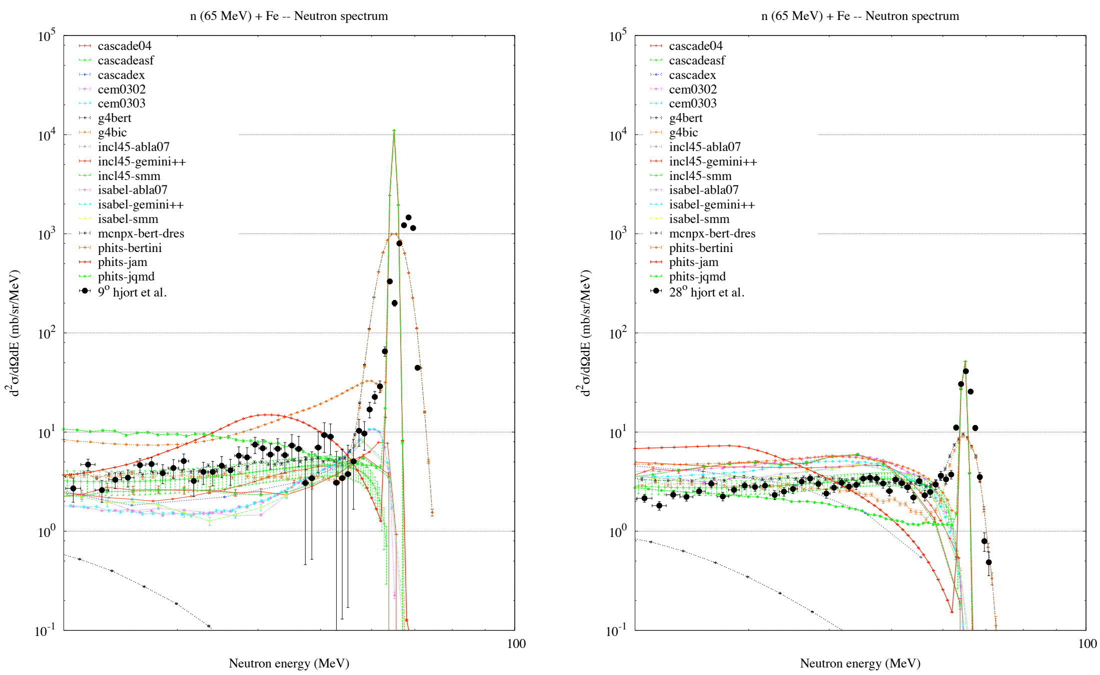


Fig. 11: Neutron spectra obtained from the reaction p(65MeV)+Fe at two angles (Θ=9° on the left and Θ=28° on the right) [xxx].

If the inelastic peak can't be produced in reactions induced by low energy projectiles, the elastic peak still exists. Fig. 11 shows this peak at 9° and 28°. Only two groups of models exhibit this peak: the three phits and the two geant4. Looking at the shape of the spectra between the peak and the lower energies in the phits case, it is clear that this peak has been added artificially. For geant4 it could be the same, but here the link

between the peak and the low energies is much smoother. The other difference is the width of this peak, which is too narrow for phits and too large for geant4.
Otherwise, forgetting the peak, all models give not so bad results, i.e. within a factor 2 and even much better, except mcnpx-bert-dres.

3.2) Transversal angles

This is the angular domain where the shape of the neutron spectrum is the best reproduced by all models. That is clearly proved by the M factors given in Fig. 12. This M factor has been described in the section "methodology" and characterizes the ability to reproduce a given shape (M must be close to zero). Thus, forward angles are difficult to fit because of the peaks and the backward angles because of the multiple scatterings.

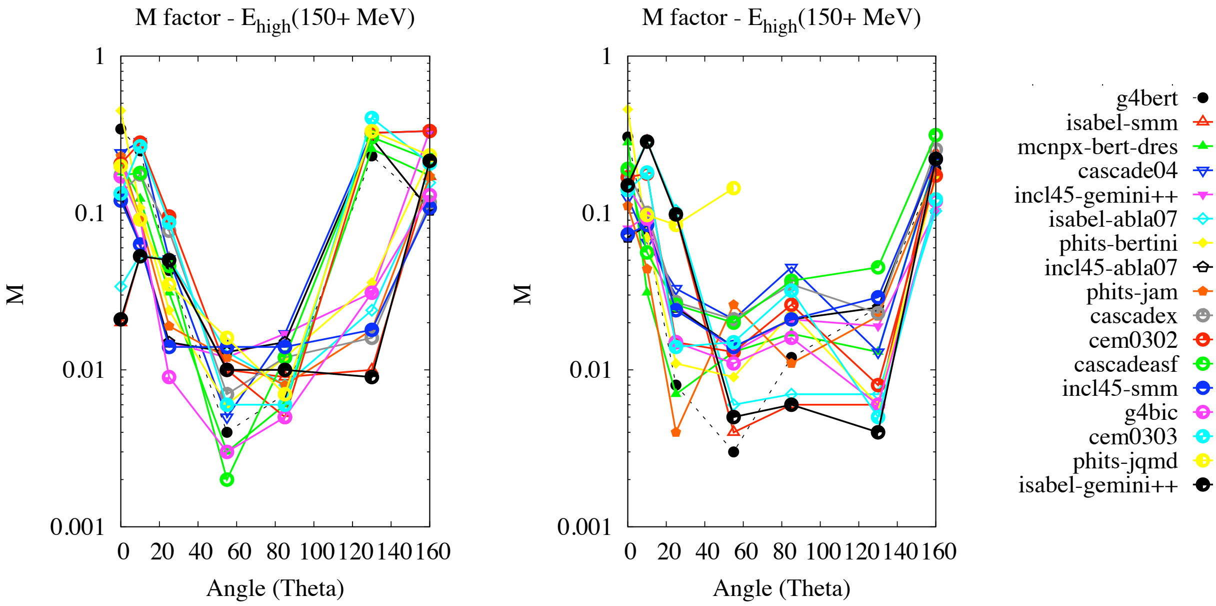


Fig. 12: M deviation factor (Intrinsic Discrepancy) dependence with angle in the high-energy region ($E_{neutron}$ > 150 MeV) for two reactions: p(800MeV)+Fe and p(1600MeV)+Pb [xxx]

However with Fig. 13 one can see that the fit is less good and the differences between the models bigger as the projectile energy and the mass target increase. Moreover, even if the results are still ok, phits-jam systematically underestimates the neutron production and INCL4.5 overestimates it. For this latter model a little shoulder appear around 200 MeV, especially in p(800MeV)+Fe. Geant4-bertini and cascadex also overestimate the results, but in specific cases: with lead for geant4-bertini and with iron at 800 MeV for cascadex. Nevertheless it seems that these under- and over-estimation disappear for a high-energy projectile (see Fig. 14).

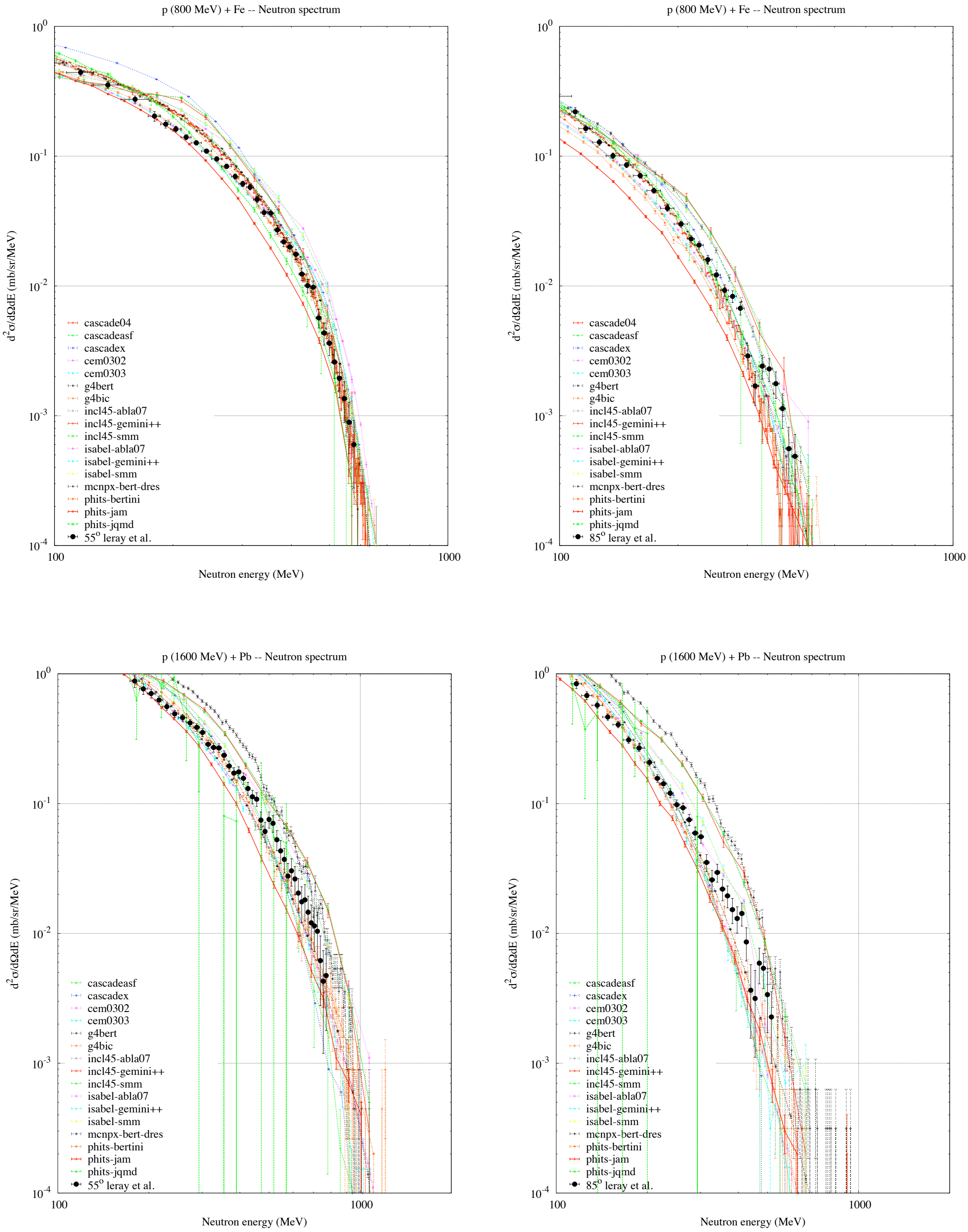


Fig. 13: Neutron spectra obtained from the reactions p(800MeV)+Fe (upper part) and p(1600MeV)+Pb (lower part) at two angles (Θ=55° on the left and Θ=85° on the right) [xxx].

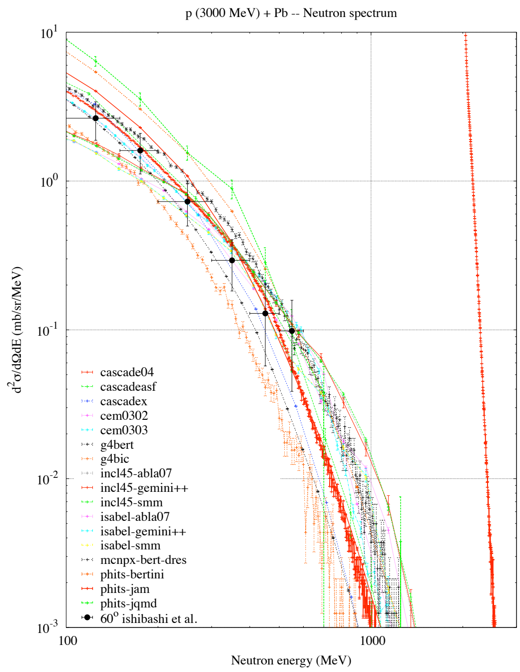


Fig. 14: Neutron spectrum obtained from the reaction p(3000MeV)+Pb at Θ=60° [xxx].

3.3) Backward angles

Spectra of high-energy neutrons at backward angles have two main features: low cross sections and fall down rapidly with energy. Even so, the models give the right shape and calculated values are within a factor 2 and even much better (Fig. 15). With a projectile energy of 800 MeV some models can fits within 10-20% (phits-jam, phits-bertini and INCL4.5).

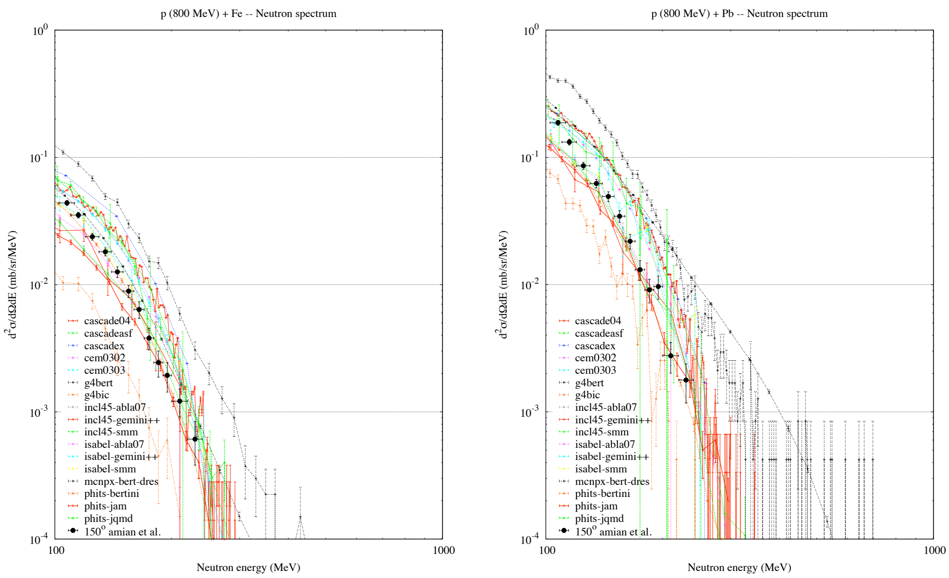


Fig. 15: Neutron spectra obtained from the reaction p(800MeV)+Fe and p(800MeV)+Pb at Θ=160° [xxx]

Too few data exist in this angular domain and Fig. 16 shows that the results seem less good when projectile energy increase and/or for more backward angles. Here all models overestimate the experimental data whereas in Fig. 15 only Geant4-bertini was too high. On the other hand, geant4-bic that underestimated the results in Fig. 15 would be the best one in Fig. 16. This region needs that the models describe the multiple scattering very well, because here all errors in the microscopic ingredients (cross sections, emission angle) can be averaged in the better case, or accumulated in the worst case.

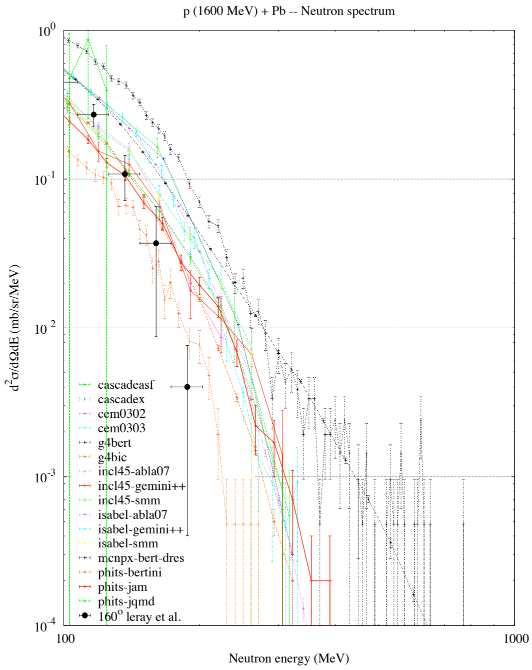


Fig. 16: Neutron spectrum obtained from the reaction p(1600MeV)+Pb at Θ=160° [xxx].

4) Each model as a whole

In the previous sections results of the models were compared to the experimental data and analysed by energy and angle to make easier a link with the physics ingredients.
But, to get an overview of the spectra the study has to be done, understood in the whole energy range and angular domain. With Fig. 17 we give an example. The model shown here clearly overestimates the low energy neutrons and fits very well the medium energy neutron at backward angles and the overall shape is rather good. So a possibility could be an overestimation of the reaction cross section, which would lead, with a better cross-section, to a good description of all energies and angles except where it was better before.
Thus a brief summary for each model is given below. First Fig. 18 shows a rating done for all data and secondly the main successes and deficiencies are pointed out.

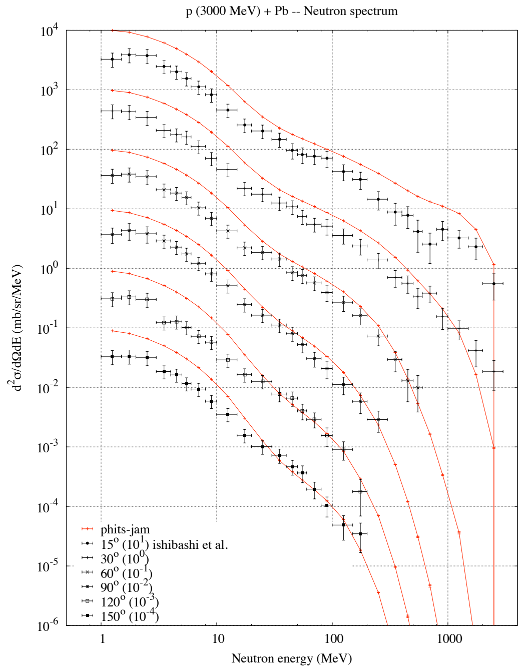


Fig. 17: Neutron spectra obtained from the reaction p(300MeV)+Pb [xxx]. The model plotted is phits-jam [xxx].

4.1) Rating

Using the rating procedure described in the section "methodology" we obtained Fig. 18. Rating goes from -2 (systematically wrong) to 2 (good with no problem). This rating shows that the neutron spectra are quite well reproduced and the differences between the models are in average not so important. Even if some models seem better than some others, we saw in the previous sections that all models can be improved in a region (energy/angle) or another.

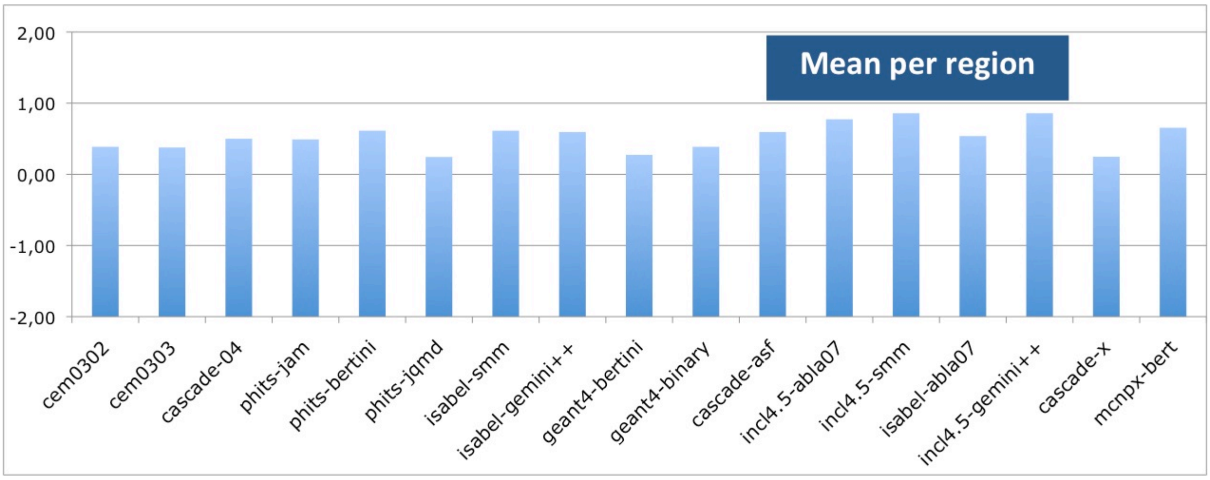


Fig. 18: Rating results for the seventeen models on neutron spectra.

4.2) Successes/Deficiencies

The table 1 points out the main qualities and shortcomings of each model.

Models	Successes	Deficiencies
cem0302	• Intermediate energy • Low projectile energy	• Peaks • Evaporation
cem0303	• Intermediate energy • Low projectile energy	• Peaks • Evaporation
cascade04	• Intermediate energy	• Peaks
cascadeasf	• Intermediate energy	• Peaks ?
cascadex		• Peaks • Evaporation
phits-bertini	• Intermediate energy	• Peaks
phits-jam	• Evaporation	• Peaks?
phits-jqmd	• Peaks	• Time consuming • Intermediate energy • Evaporation
geant4-bertini		• Peaks (no inelastic??? - elastic: too low/high (0°/25°) • High energy
geant4-bic	• Peaks (one of the best model - inelastic a little bit too large)	• High energy (except peaks)
mcnpx-bert-dres		• Peaks 0° • Evaporation • No more improved
incl45-abla07	• High energy (peaks included)	• Intermediate energy • depression at 10 MeV (low projectile energy)
incl45-smm	• High energy (peaks included) • Evaporation	• Intermediate energy • depression at 10 MeV (low projectile energy)
incl45-gemini++	• High energy (peaks included) • Evaporation	• Intermediate energy • depression at 10 MeV (low projectile energy)
isabel-abla07	• Inelastic Peak	• Intermediate energy
isabel-smm	• Inelastic Peak • Evaporation	• Intermediate energy
isabel-gemini++	• Inelastic Peak • Evaporation	• Intermediate energy