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Title: The MCNP6 Event Generator CEM03.02: Lessons Learned from the Intercomparison

Author(s): Stepan G. Mashnik, Arnold J. Sierk, Konstantin K. Gudima, and Mircea I. Baznat

Intended for: Viewgraphs for the invited talk to be presented at the Second Advanced Workshop on Model Codes for Spallation Reactions, CEA-Saclay, France, February 8-11, 2010

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Abstract of the invited talk to be presented at the
Second Advanced Workshop on Model Codes for Spallation Reactions,
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The MCNP6 Event Generator CEM03.02: Lessons Learned from the Intercomparison

Stepan G. Mashnik and Arnold J. Sierk

Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Konstantin K. Gudima and Mircea I. Baznat

Institute of Applied Physics, Academy of Science of Moldova, Chişinău, Moldova

Following an increased interest in intermediate-energy nuclear data for several applications, the US Department of Energy has supported during the last decade our work on the development of improved versions of the Cascade-Exciton Model (CEM) which has led to our event generator CEM03.02 used by the latest version of the LANL transport code MCNP6. We have participated with CEM03.02 and with the very similar version CEM03.03, used as an event generator in MARS15, in the Benchmark of Spallation Models organized under the auspices of the International Atomic Energy Agency during 2008 – 2009. We have discussed part of our results at the Satellite Meeting **"Nuclear Spallation Reactions"** of the *Accelerator Applications conference (AccApp'09)* held in Vienna in May 2009. Here, we present a review of our final results and lessons learned from this Intercomparison, trying to understand the reasons for the success or deficiency of CEM03.02 to describe the reactions covered by the Benchmark and to identify possible ways of futher improvements of CEM03.02 for specific needs by MCNP6. On the whole, CEM03.02 describes reasonably well most of the tested reactions. Therefore, it can be employed with confidence as a reliable event generator in MCNP6 as the main "workhorse" for intermediate-energy applications. However, the Benchmark identified several problems to be solved to improve the predictive power of CEM03.02 (and CEM03.03). Open questions on reaction mechanisms and future necessary work are outlined.

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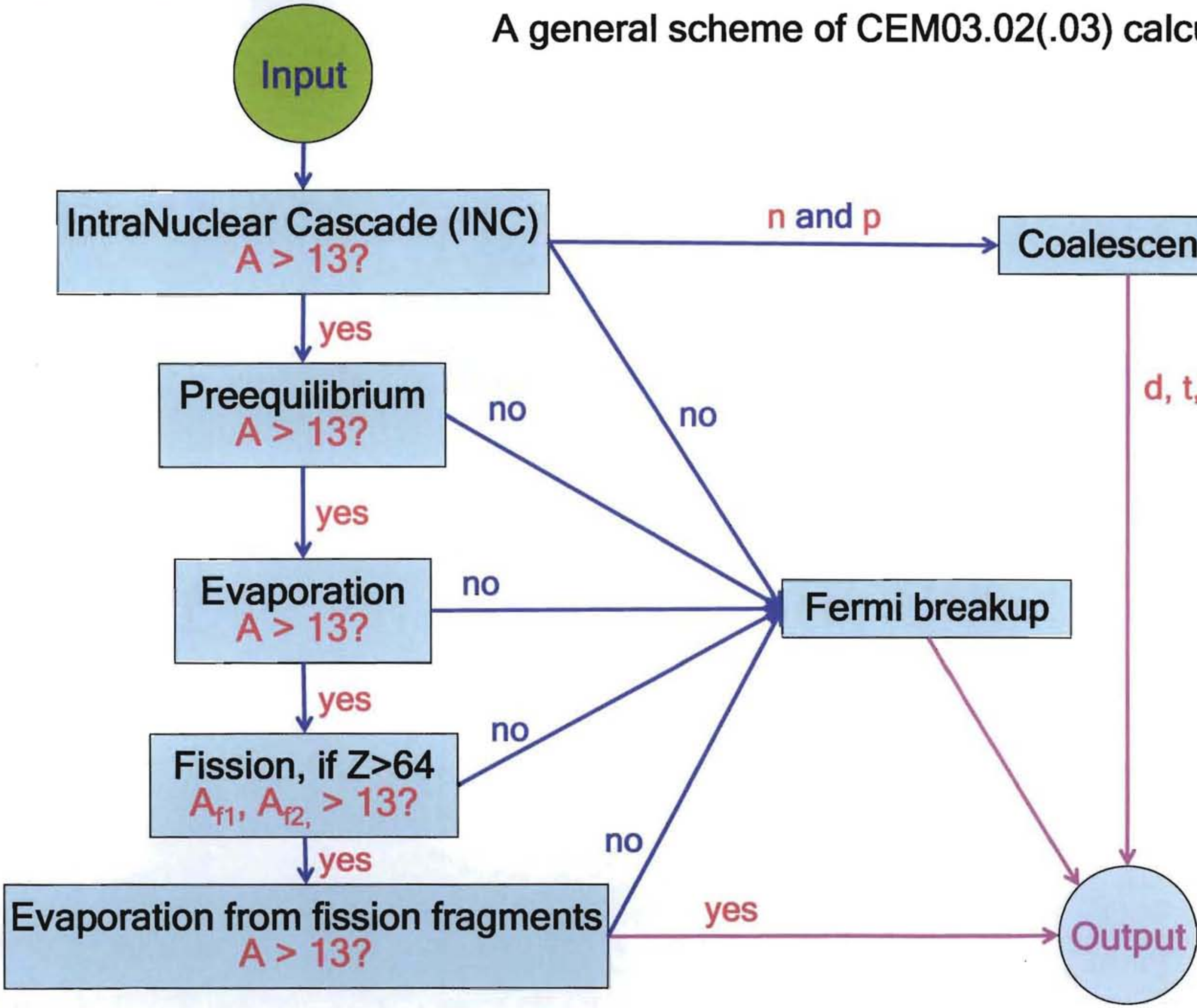
CEM03.02(.03) is 5 years old; not fit to Intercomparison data

- A general scheme of CEM03.02(.03) calculation
- Results on neutron spectra and multiplicities
- p, d, t, ^{3}He, and ^{4}He spectra from p- and n-induced reactions
- Pion spectra
- Integrated mass and charge distributions of product yields
- Mass distributions for separate isotopes
- Isotopic excitation functions
- General comments, summary

A general scheme of CEM03.02(.03) calculations



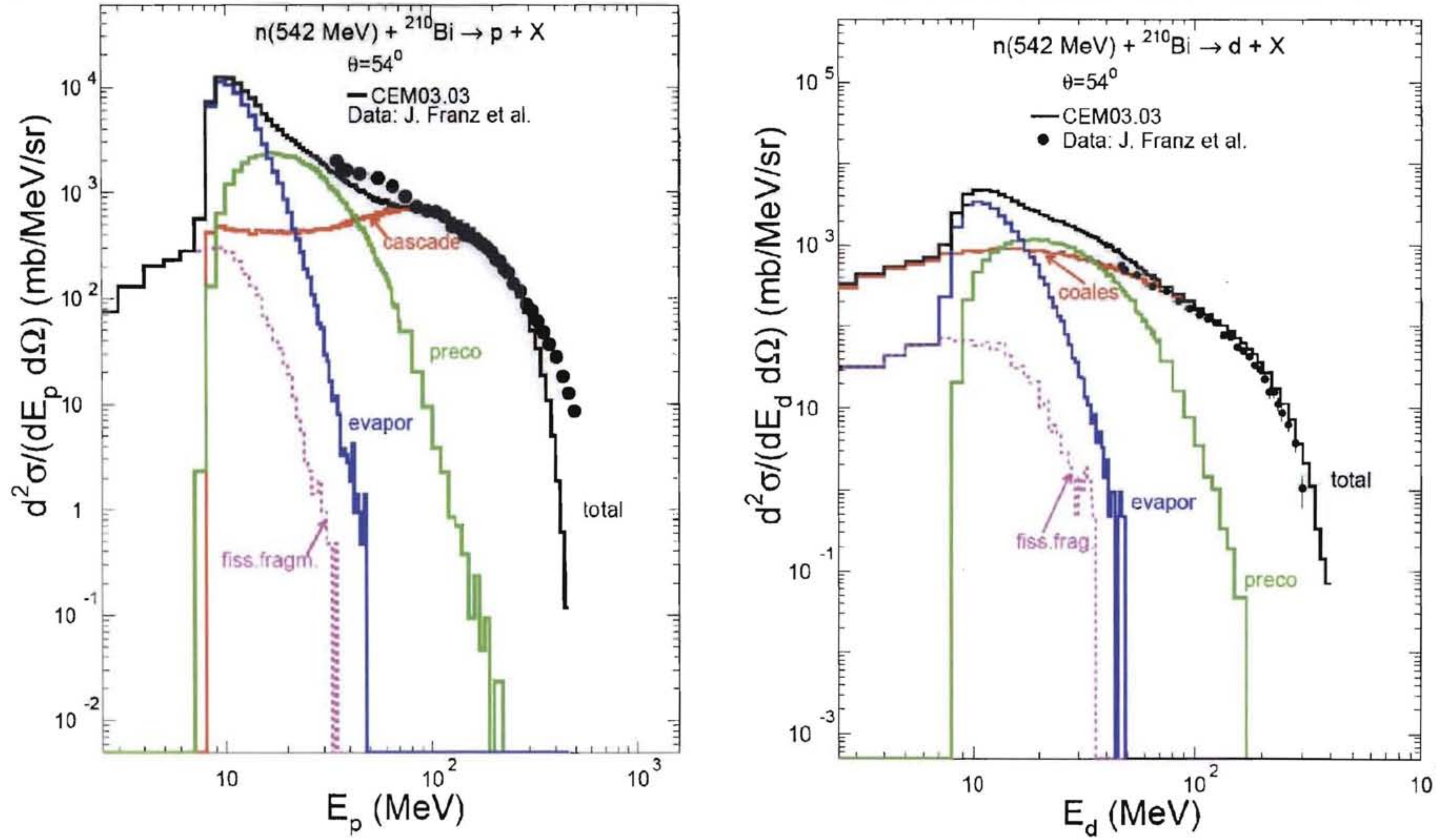
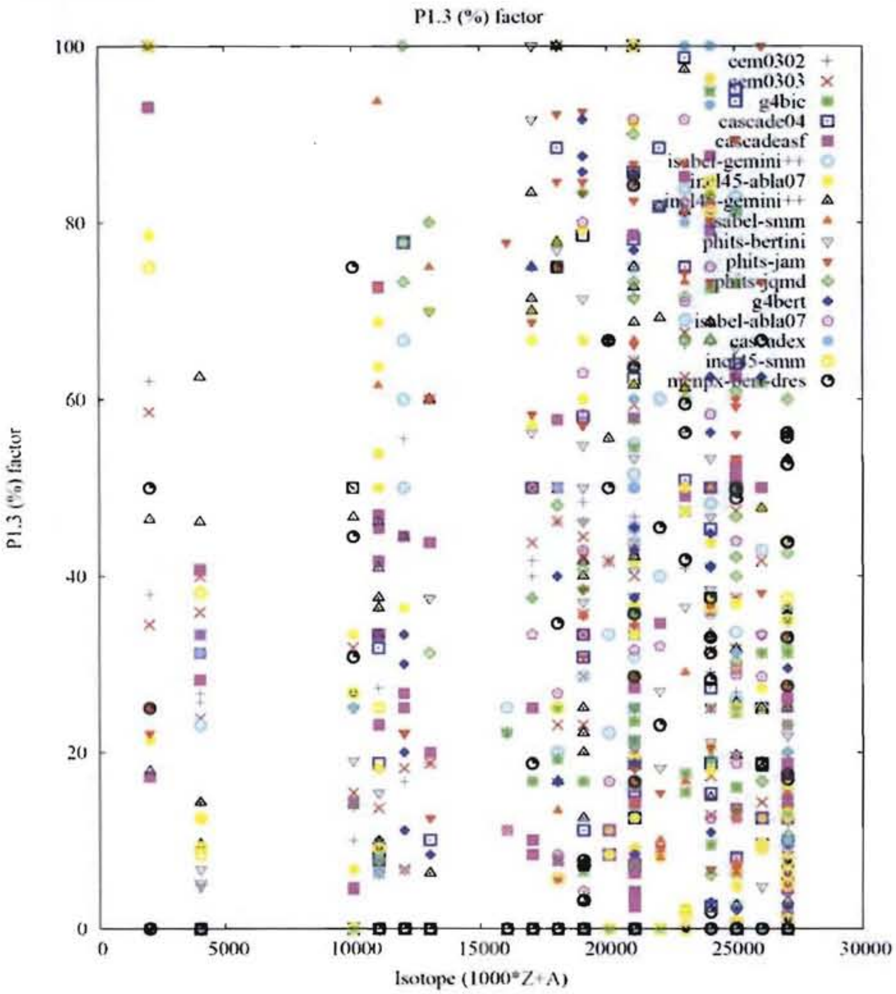
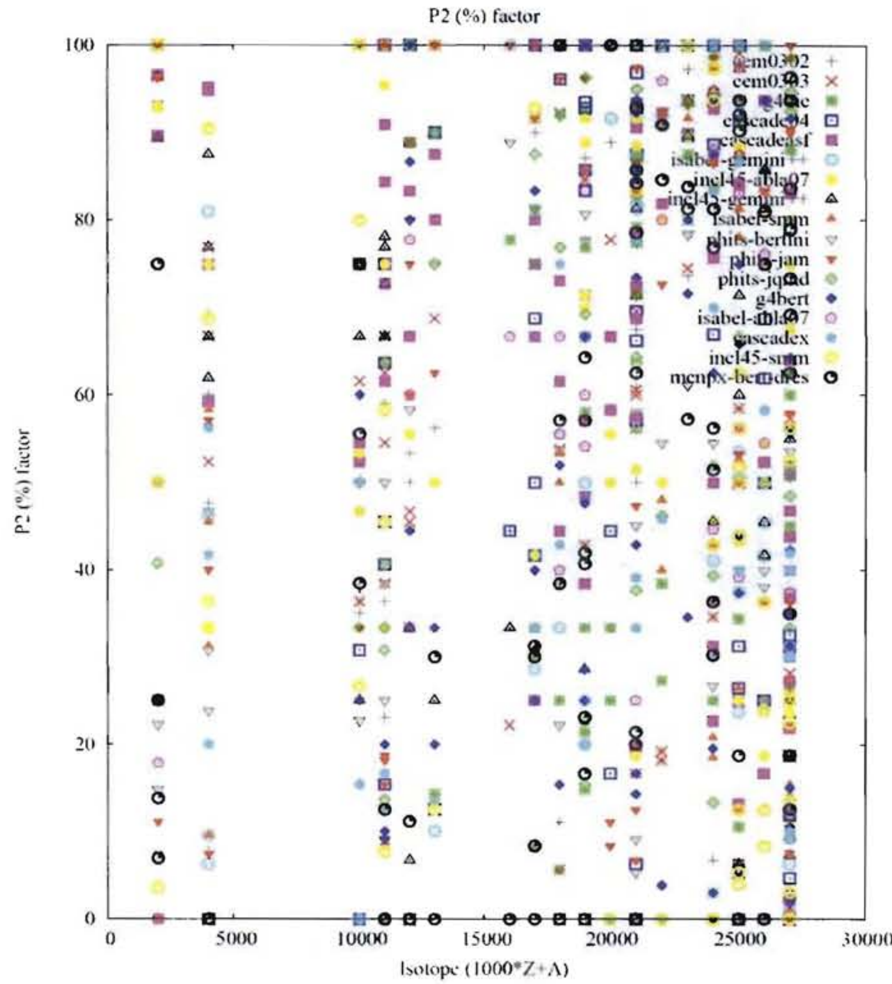
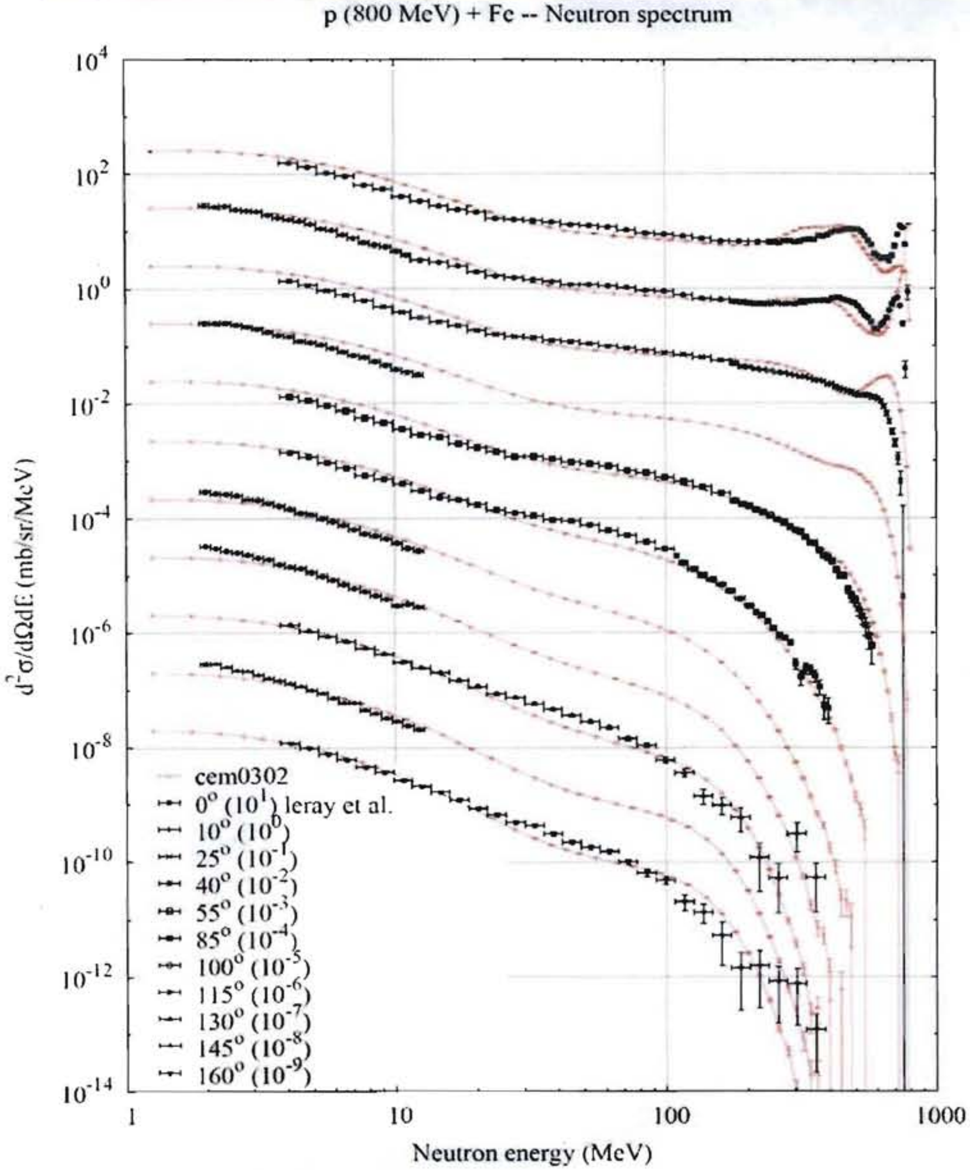


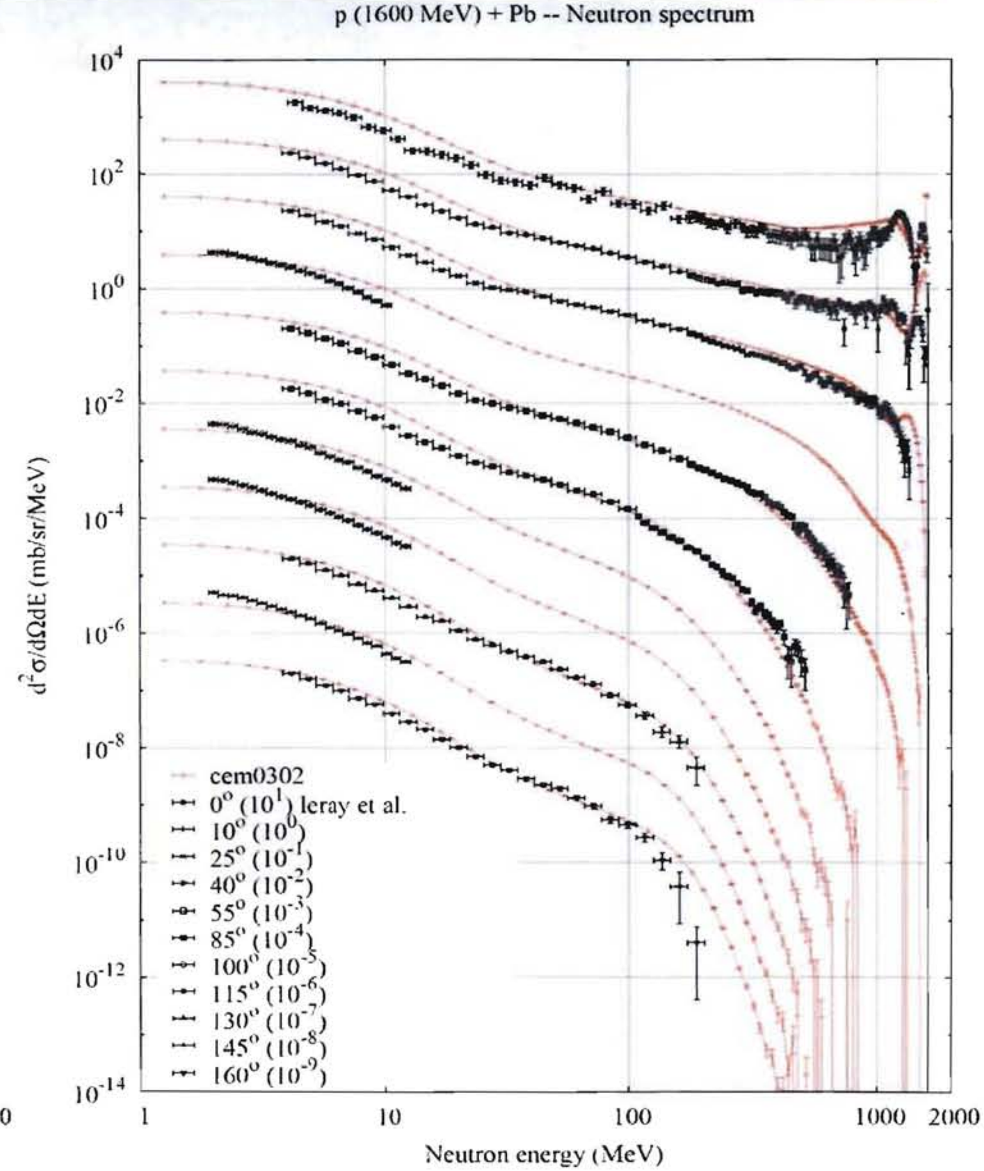
Figure 4: Experimental double-differential spectra of protons and deuterons at 54 degrees from 542 MeV n + Bi (black circles) [13] compared with our results by CEM03.03 (histograms) presented at the Benchmark [10]. Contributions from intra-nuclear cascade, preequilibrium, evaporation before or without fission, coalescence, and evaporation from fission fragments to the total spectra (black histograms) are shown by different colors, as indicated.



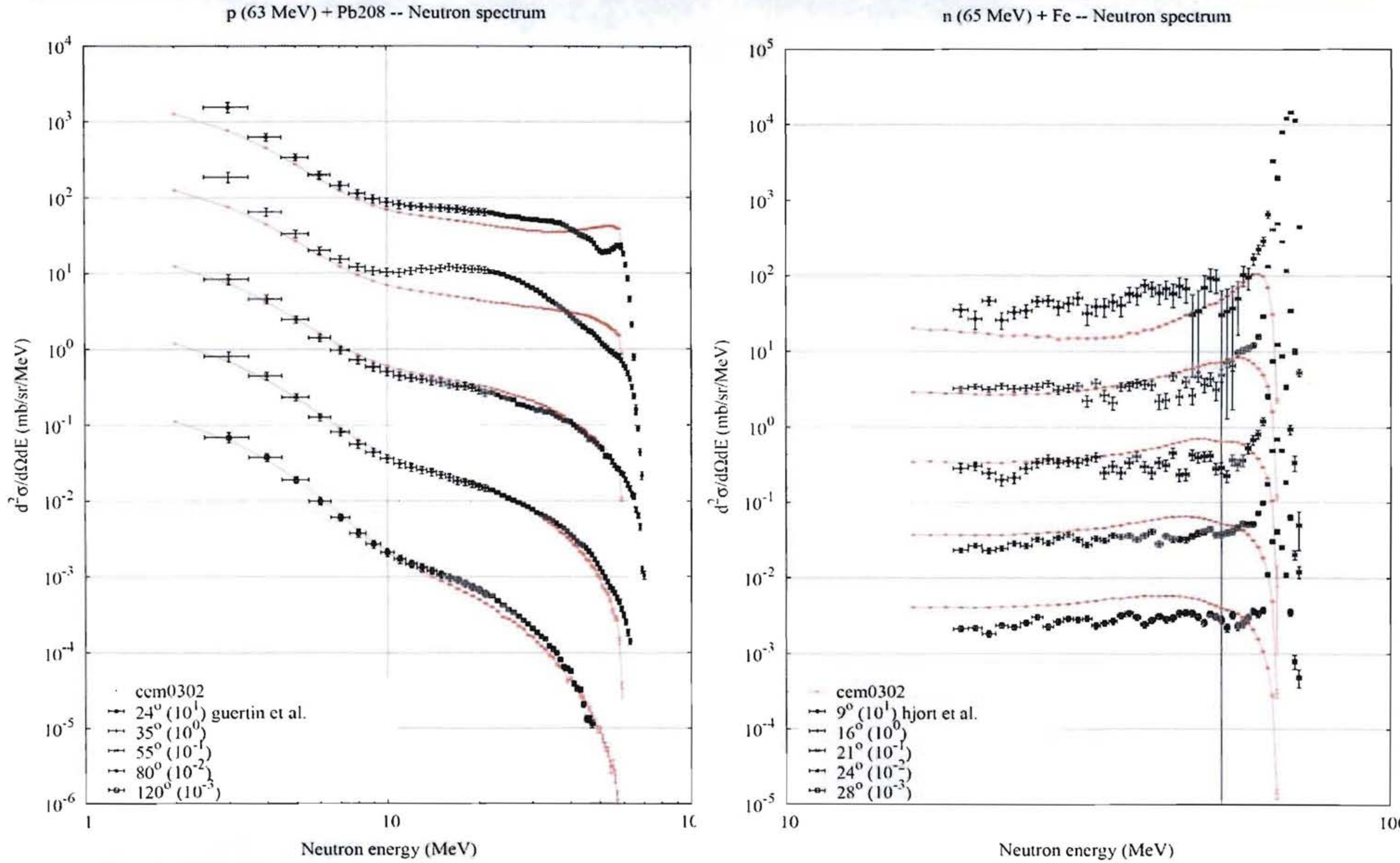


Occasionally, for some reactions, some figures of merit look more like a nice tapestry rather than a fast informative evaluation of model predictive powers; therefore we often prefer to look directly at plots with results rather than analyzing different figures of merit

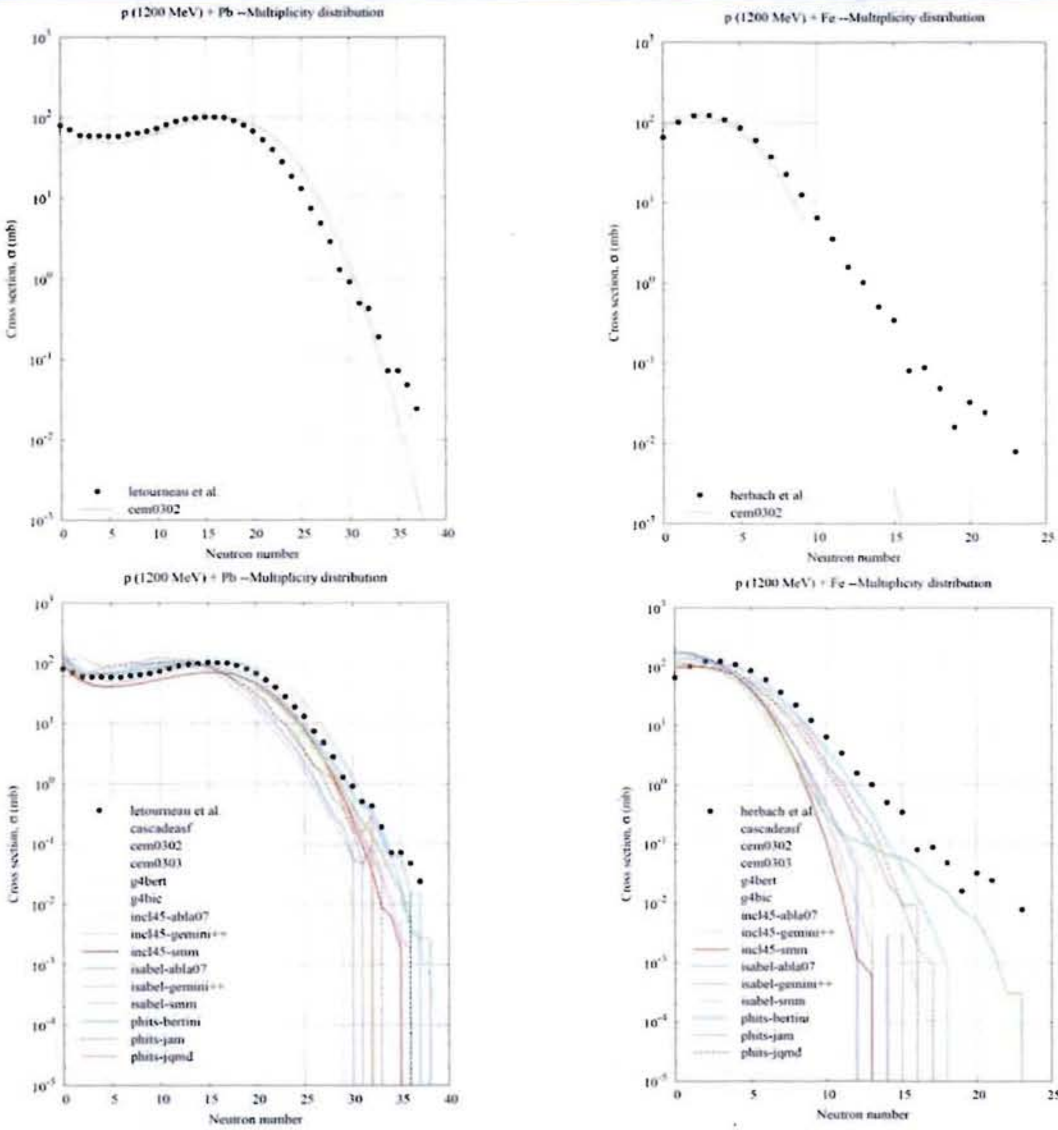




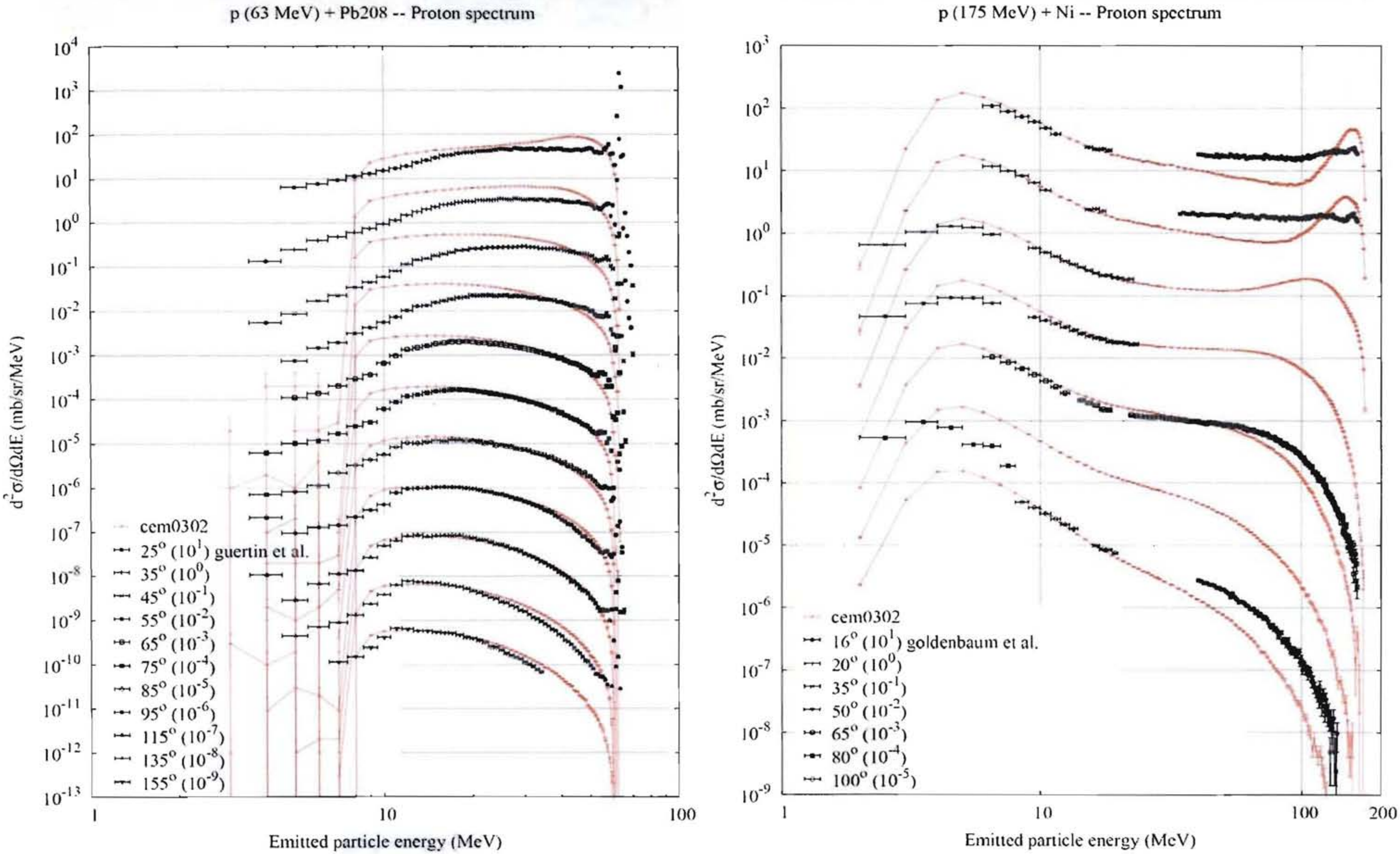
CEM03.02(03.03) describes quite well most of the neutron spectra covered by the Intercomparison



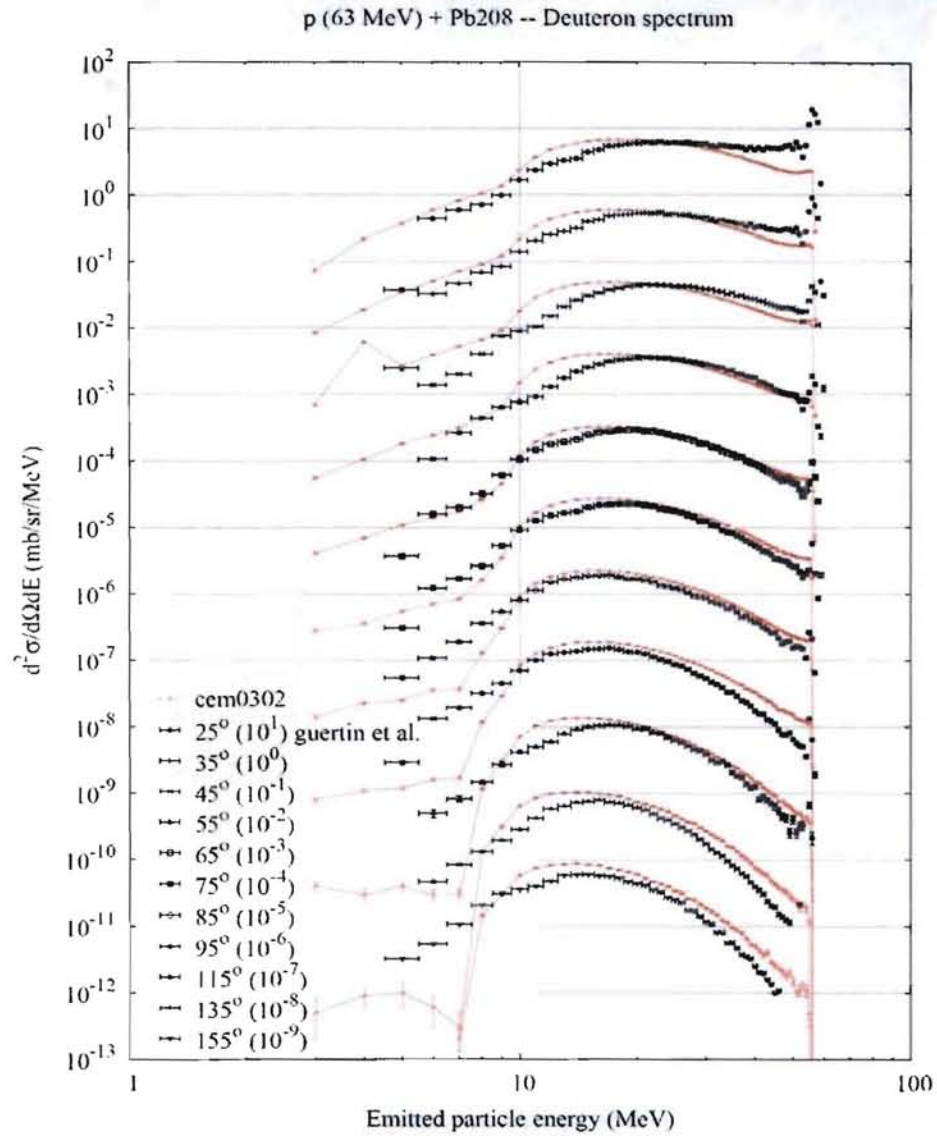
However, CEM03.02(.03) still has room for improvement of neutron spectra, especially at T < 100 MeV; we work now on this problem

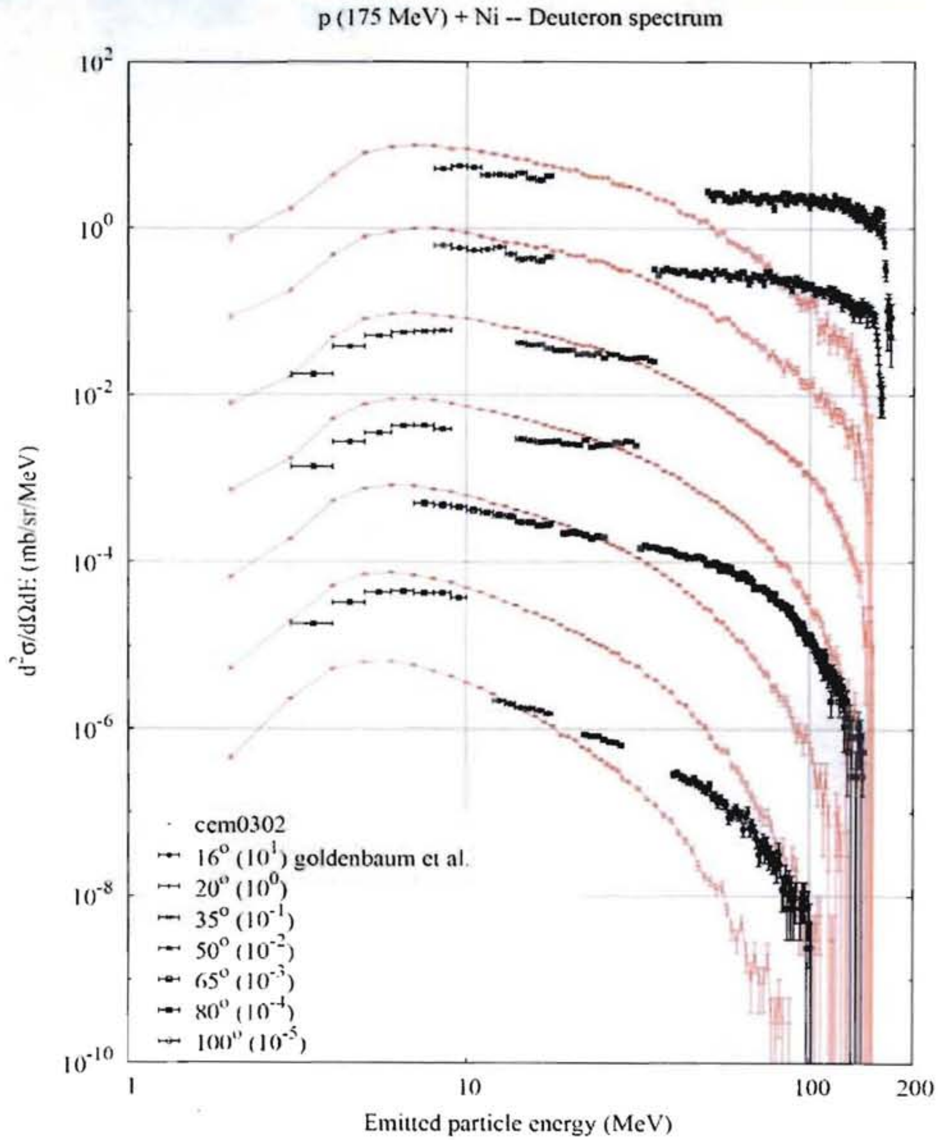


CEM03.02(.03) reproduces well the Letourneau et al. n-multiplicity distribution for 1.2 GeV p + Pb but does not agree so well with the Herbach et al. data for 1.2 GeV p + Fe, just as most other codes do for high values of <n> for this reaction

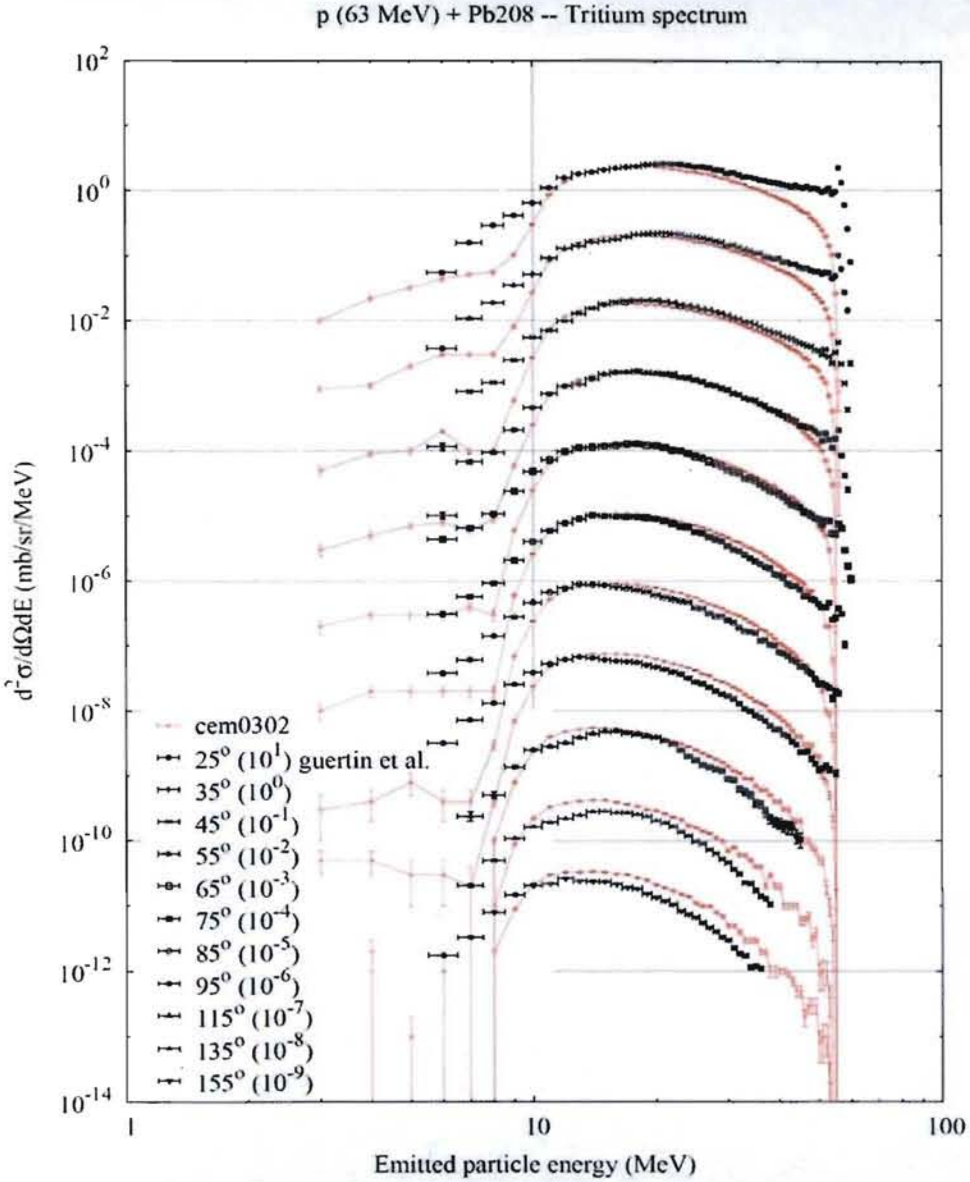


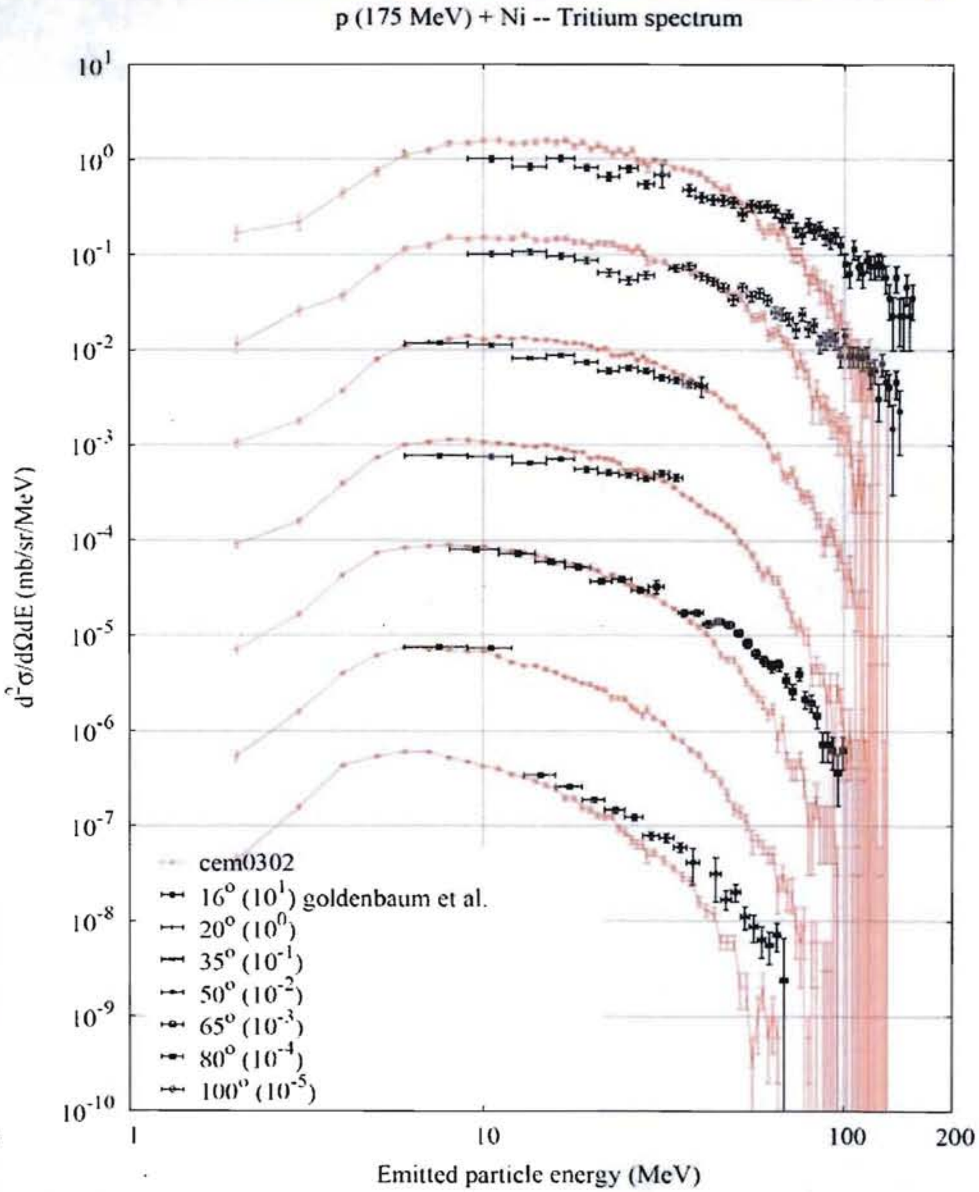
CEM03.02(.03) reproduces quite well most of the proton spectra covered by the Benchmark, though there are still some problems to be solved



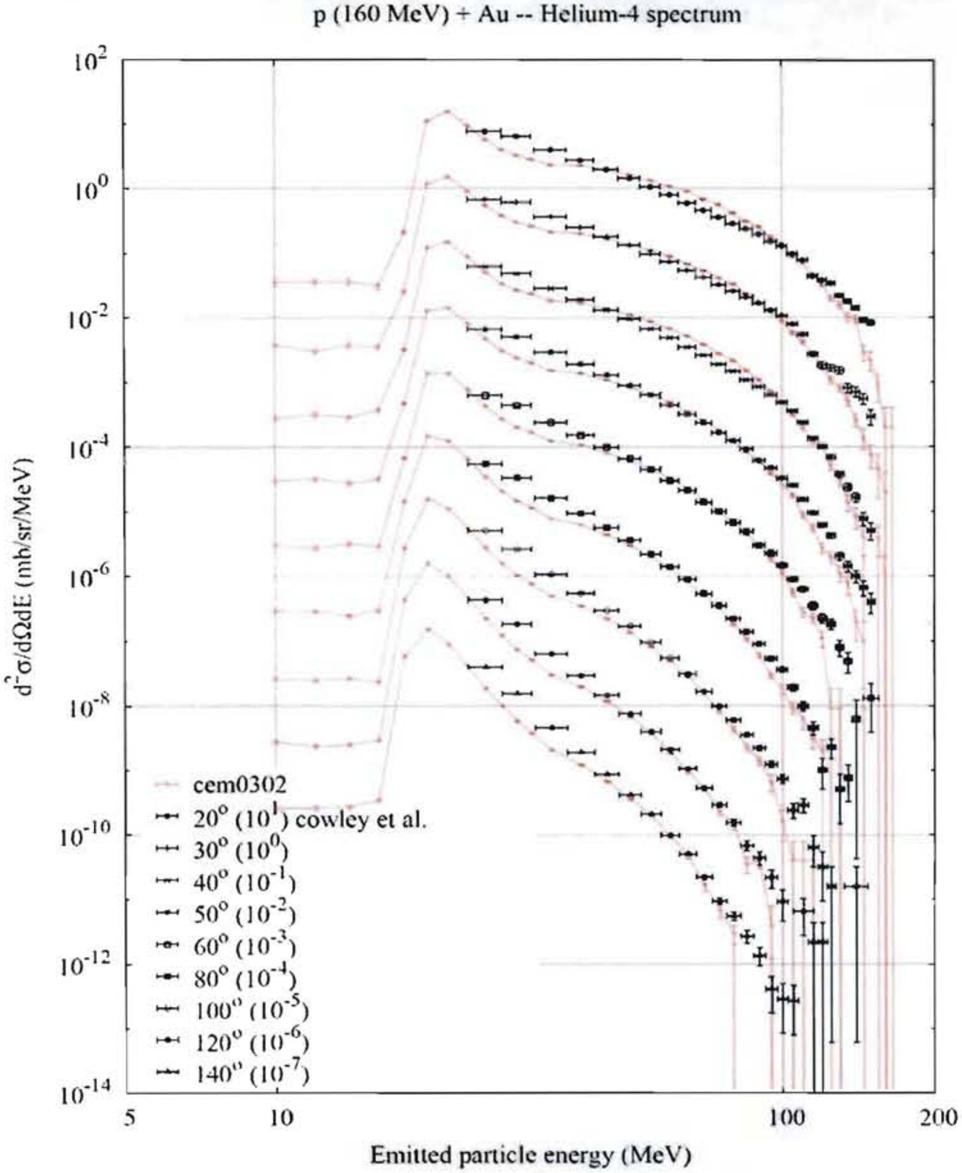


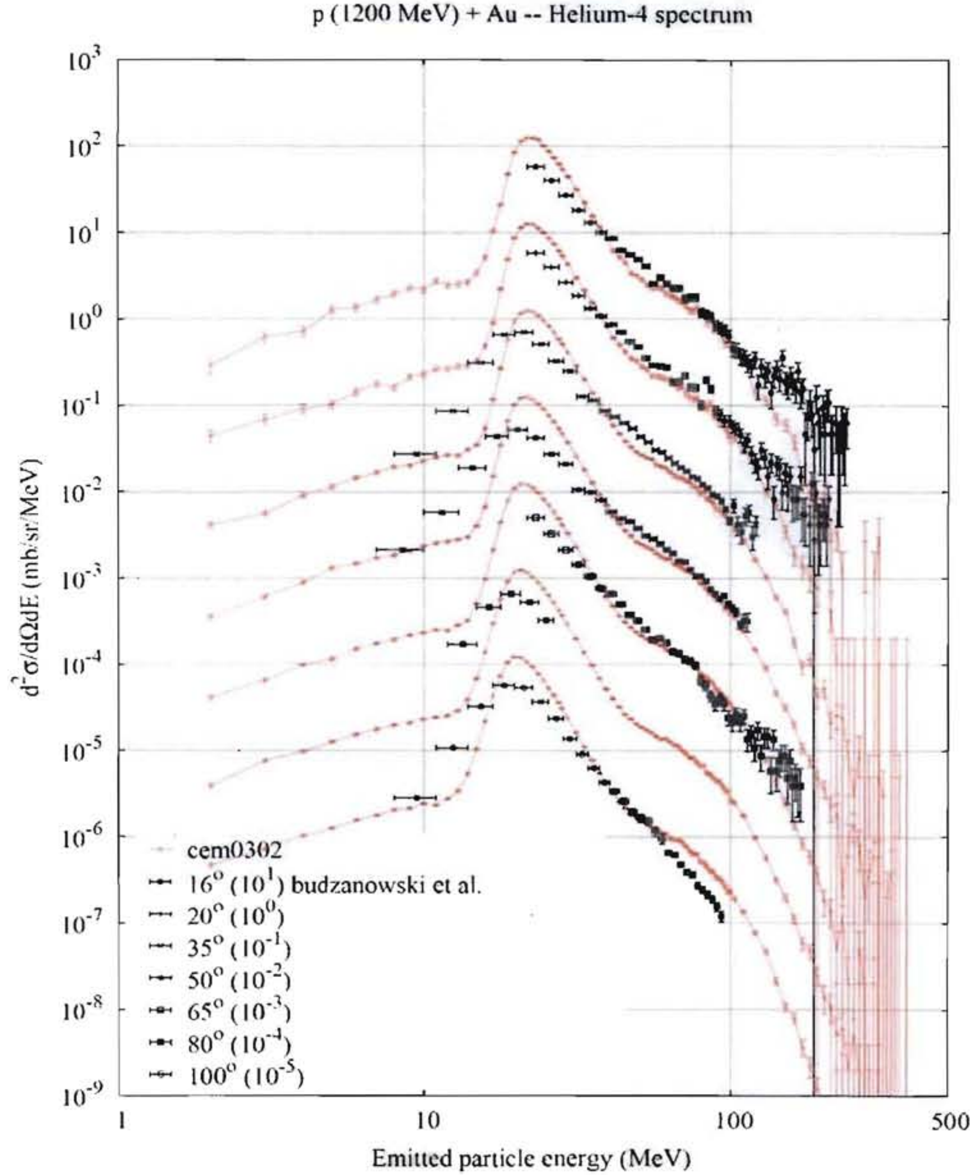
CEM03.02(.03) describes quite well also most of the deuteron spectra, though in its present version it does not account for direct processes like pick-up and knock out



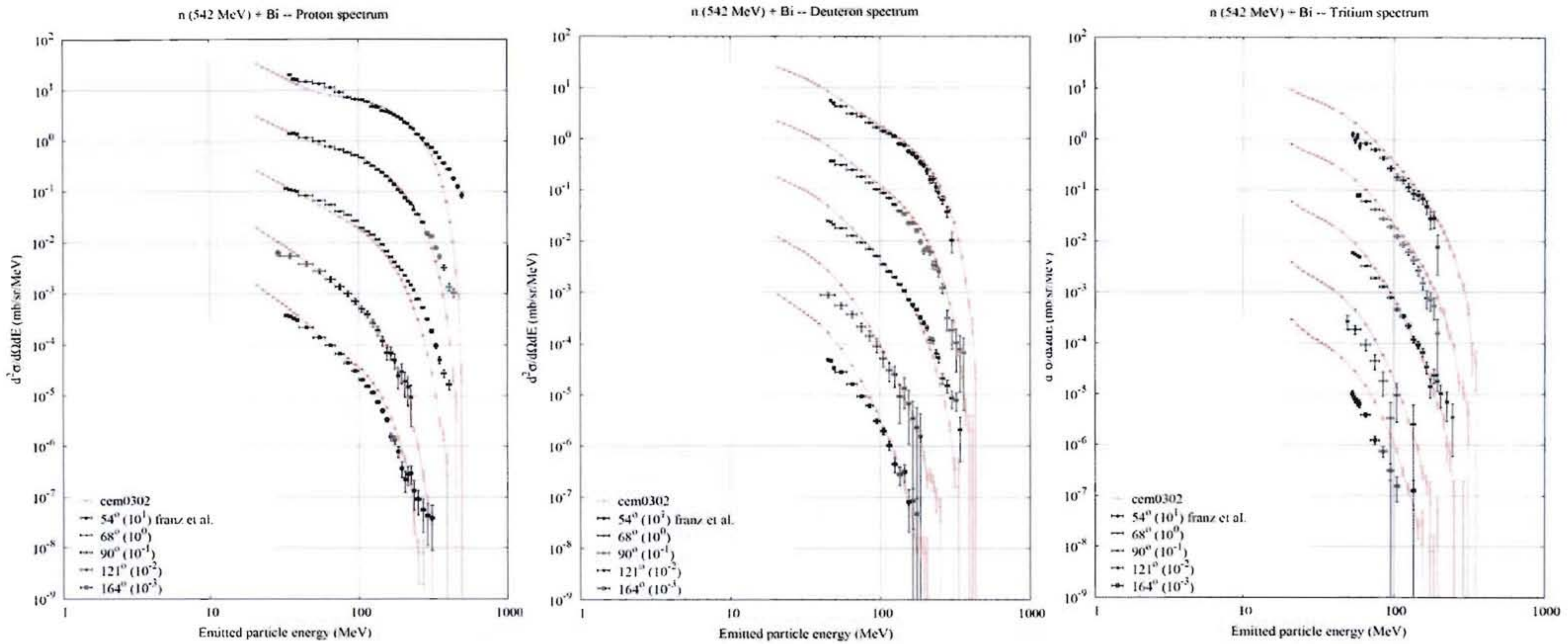


Most of the tritium spectra are also described quite well by CEM03.02(.03); very similar results are obtained for ^{3}He spectra





CEM03.02(.03) describes reasonably well most of the ^{4}He-spectra but has room for further improvement

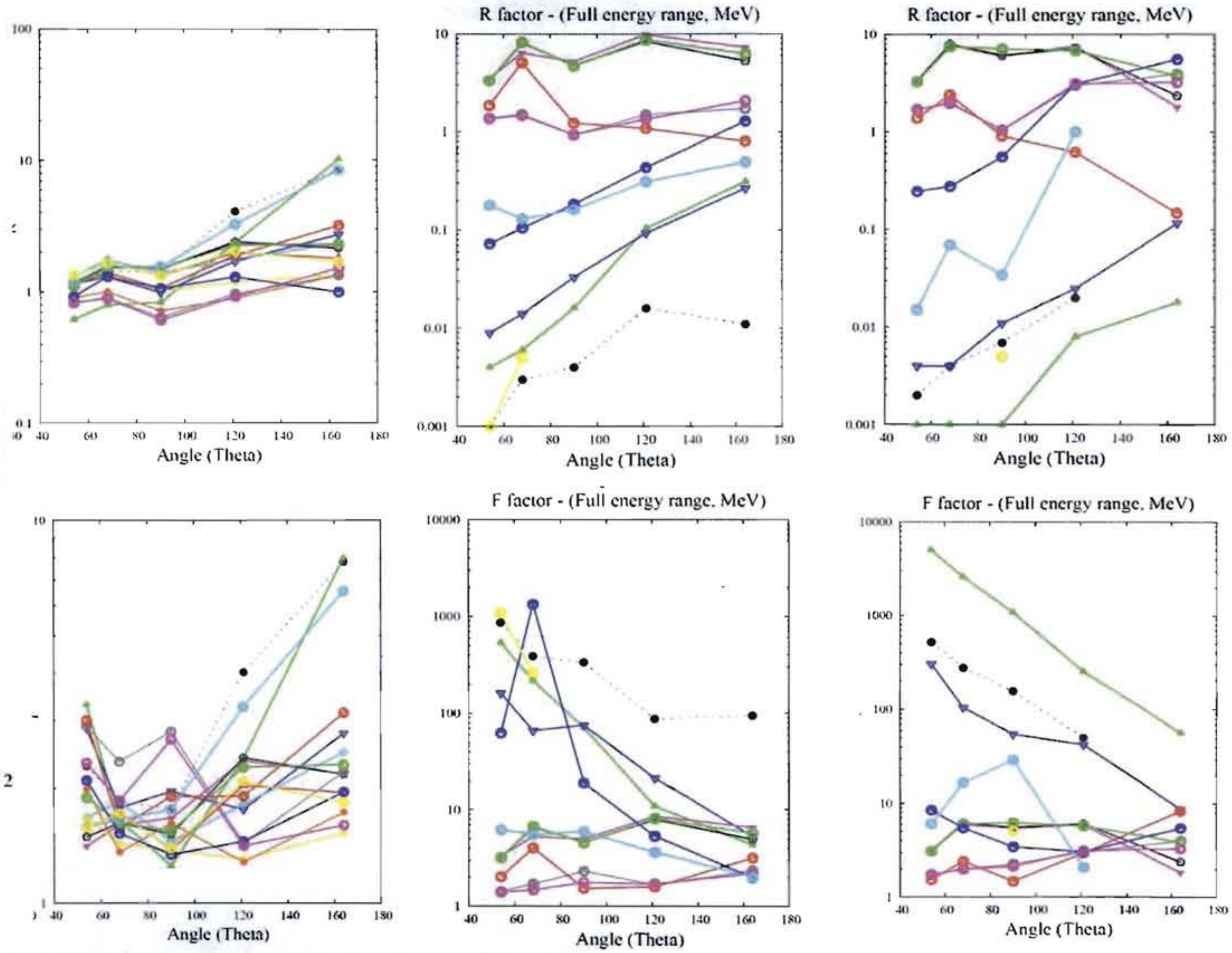


CEM03.02(.03) describes proton and complex-particle spectra from reactions induced by neutrons quite well

n (542 MeV) + Bi -- Proton spectrum   n (542 MeV) + Bi -- Deuteron spectrum   n (542 MeV) + Bi -- Tritium spectrum

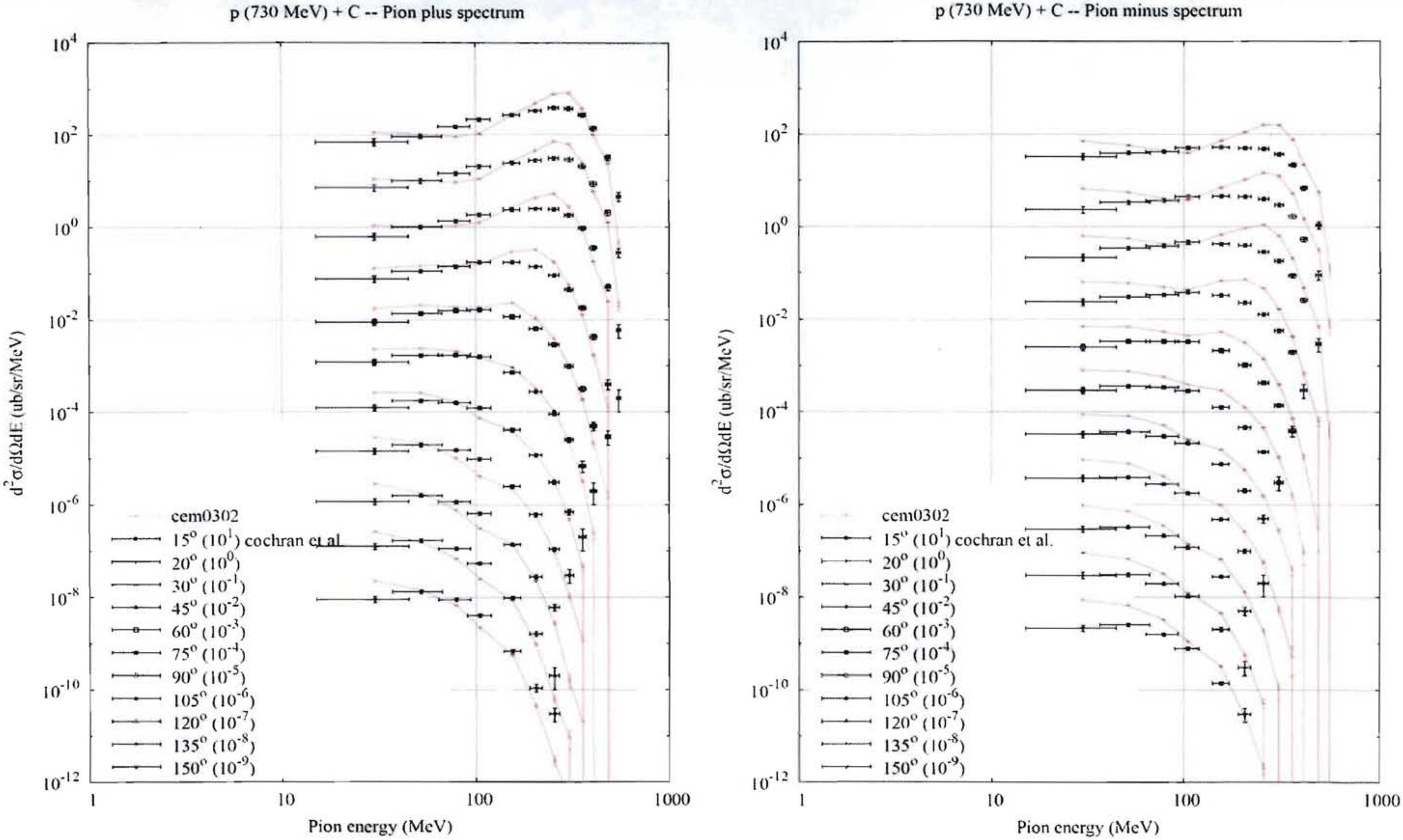
$$R = N^{-1}\sum_{i=1}^{N}\sigma_i^{calc} / \sigma_i^{\exp}$$

g4bert
mcnpx-bert-dres
cascade04
incl45-gemini++
incl45-abla07
cem0302
cascadeasf
incl45-smm
g4bic
cem0303
phits-jqmd
isabel-gemini++

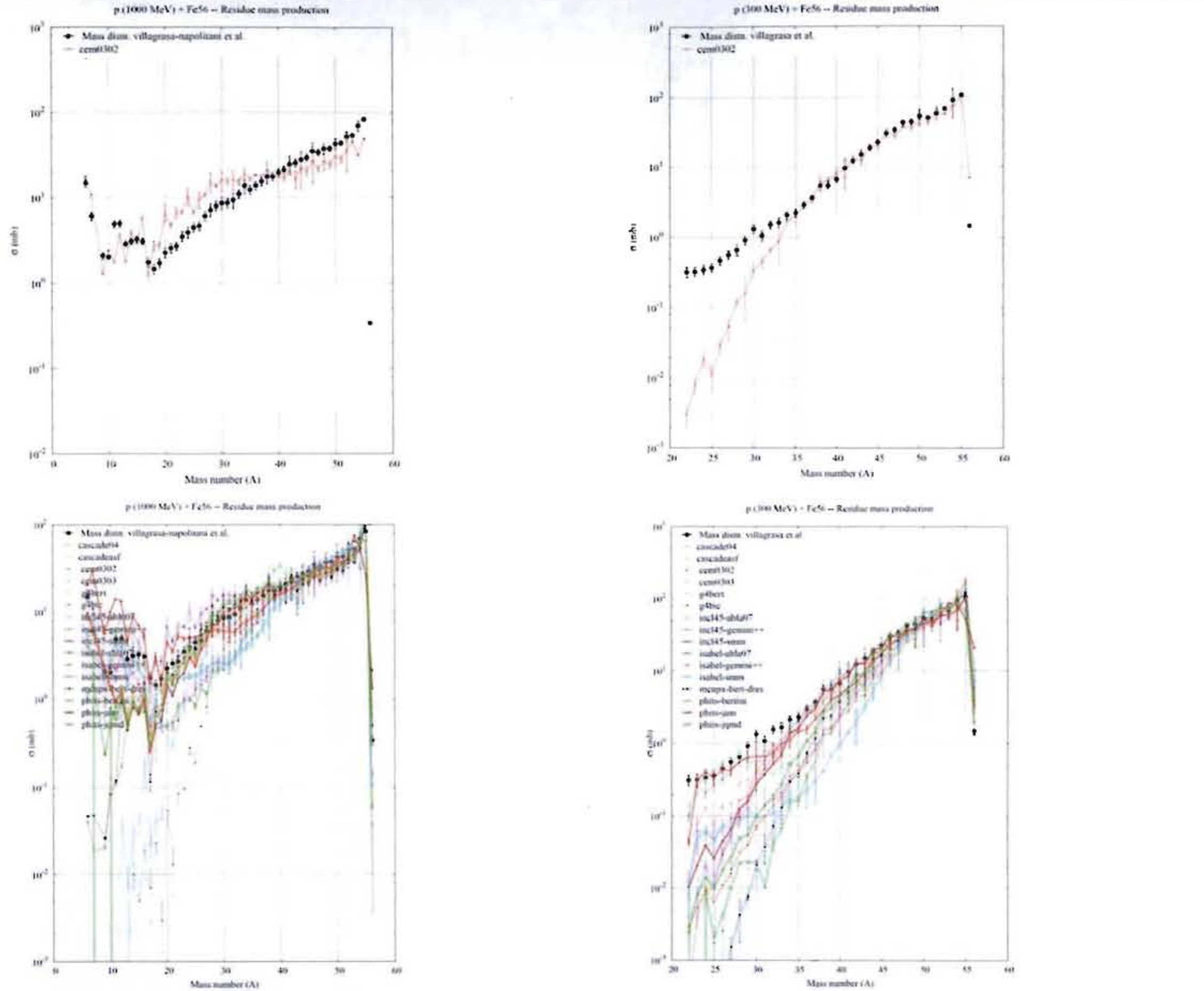


$$F = 10^{\left(N^{-1}\sum_{i=1}^{N}\left[\log(\sigma_i^{exp}) - \log(\sigma_i^{calc})\right]^2 \right)^{1/2}}$$

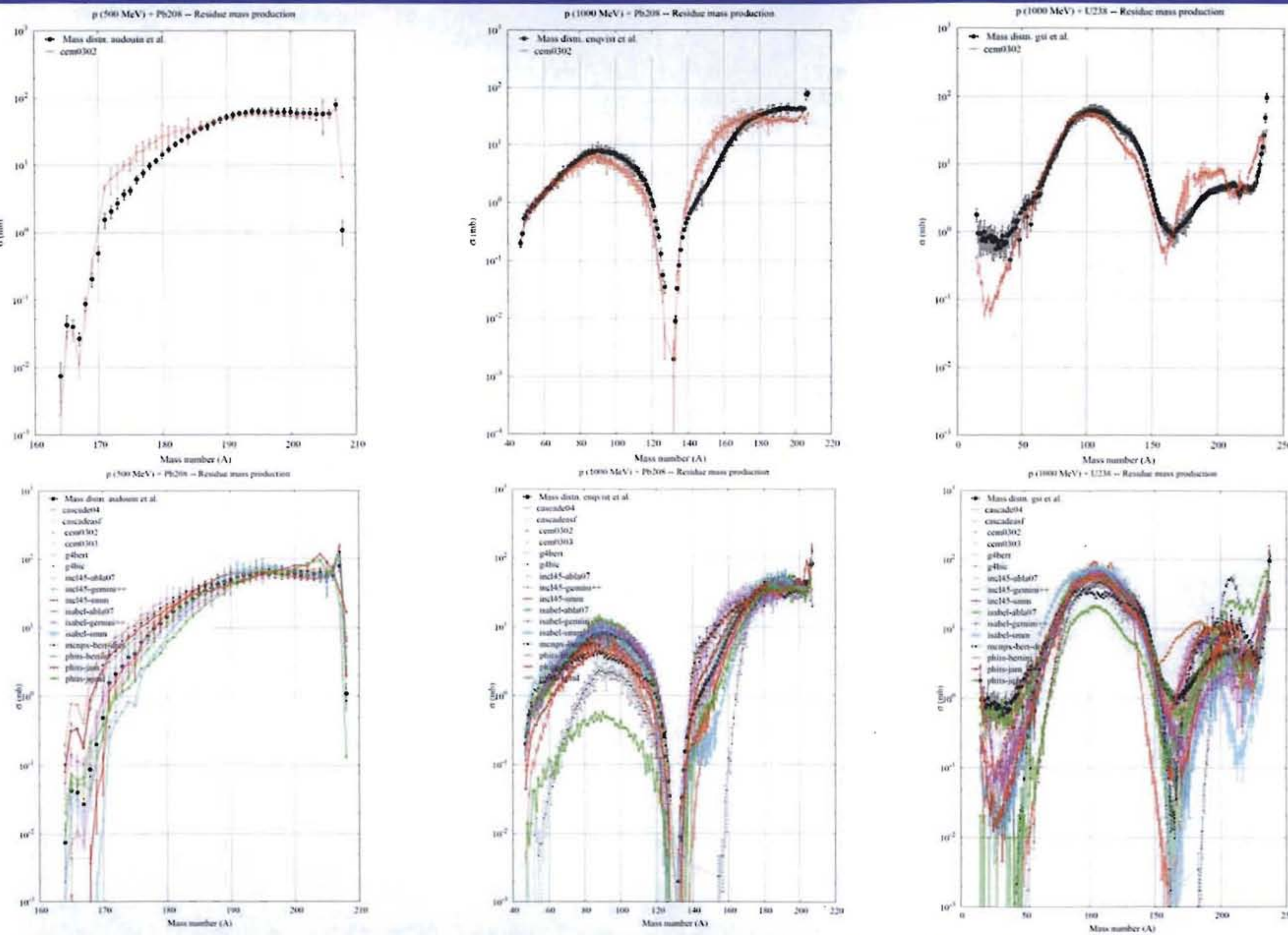
CEM03.02(.03) provides for these spectra one of the best figures of merit



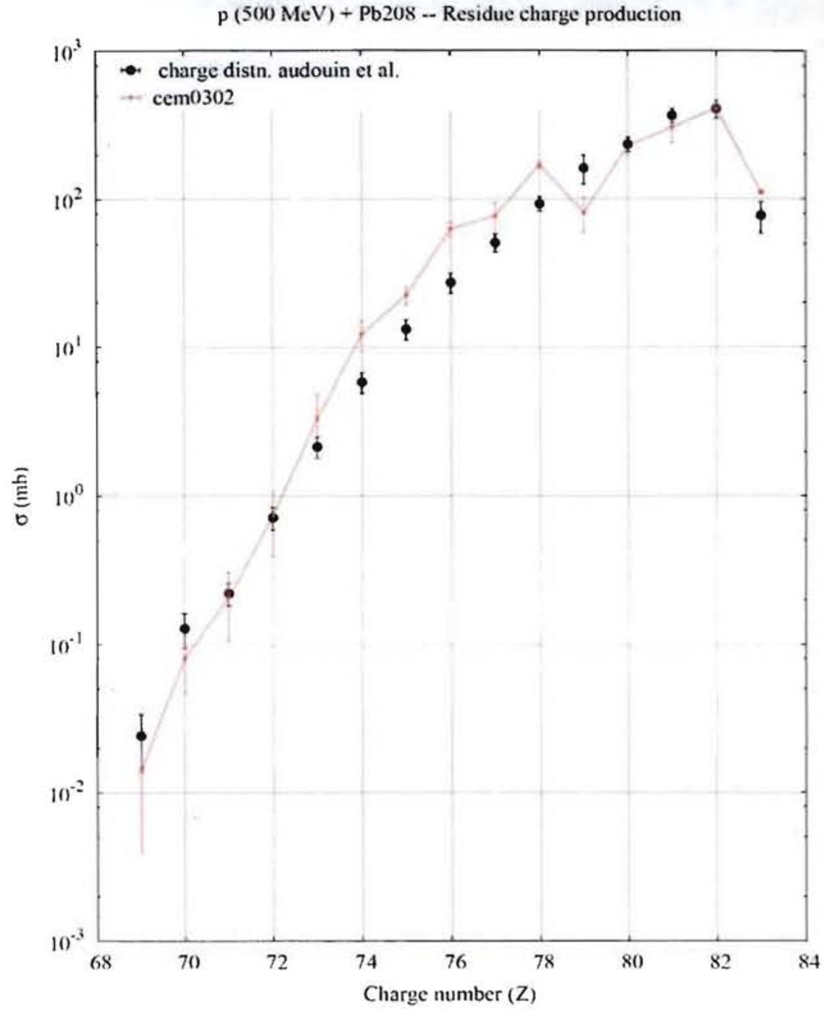
CEM03.02(.03) describes reasonably well most of the pion spectra but has room for further improvements

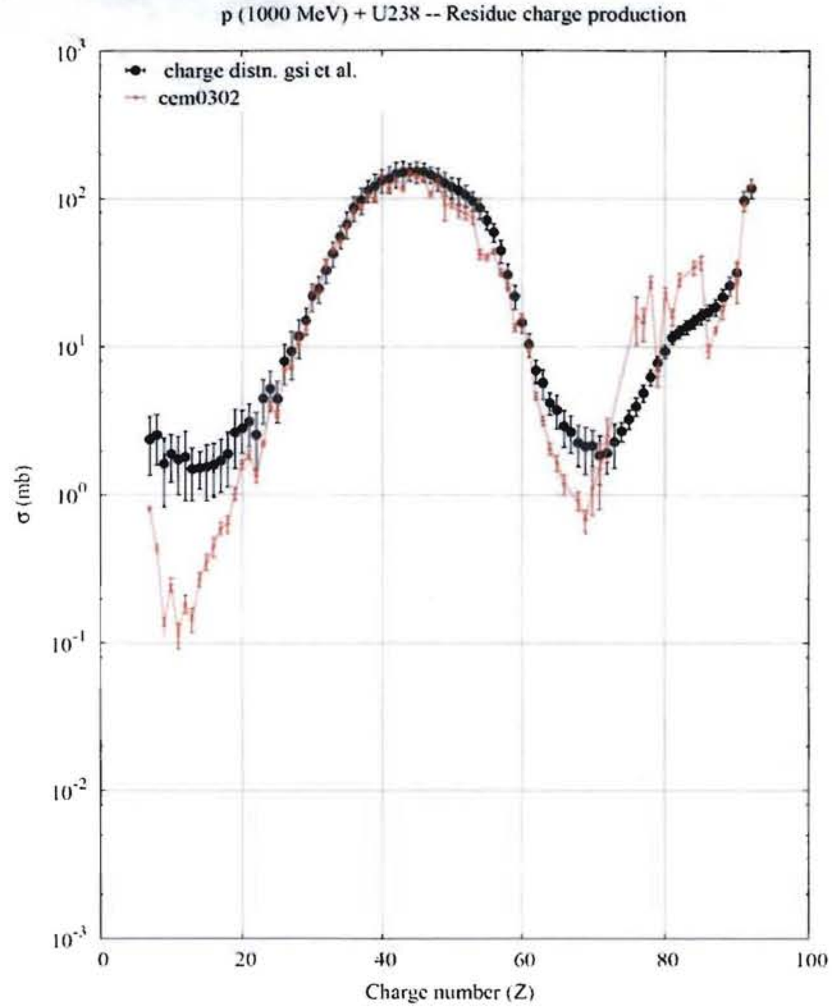


CEM03.02(.03) describes quite well the mass distribution of product yields from 1 GeV p + Fe but underestimates production of fragments with A < 30 at 300 MeV, just as most other models do

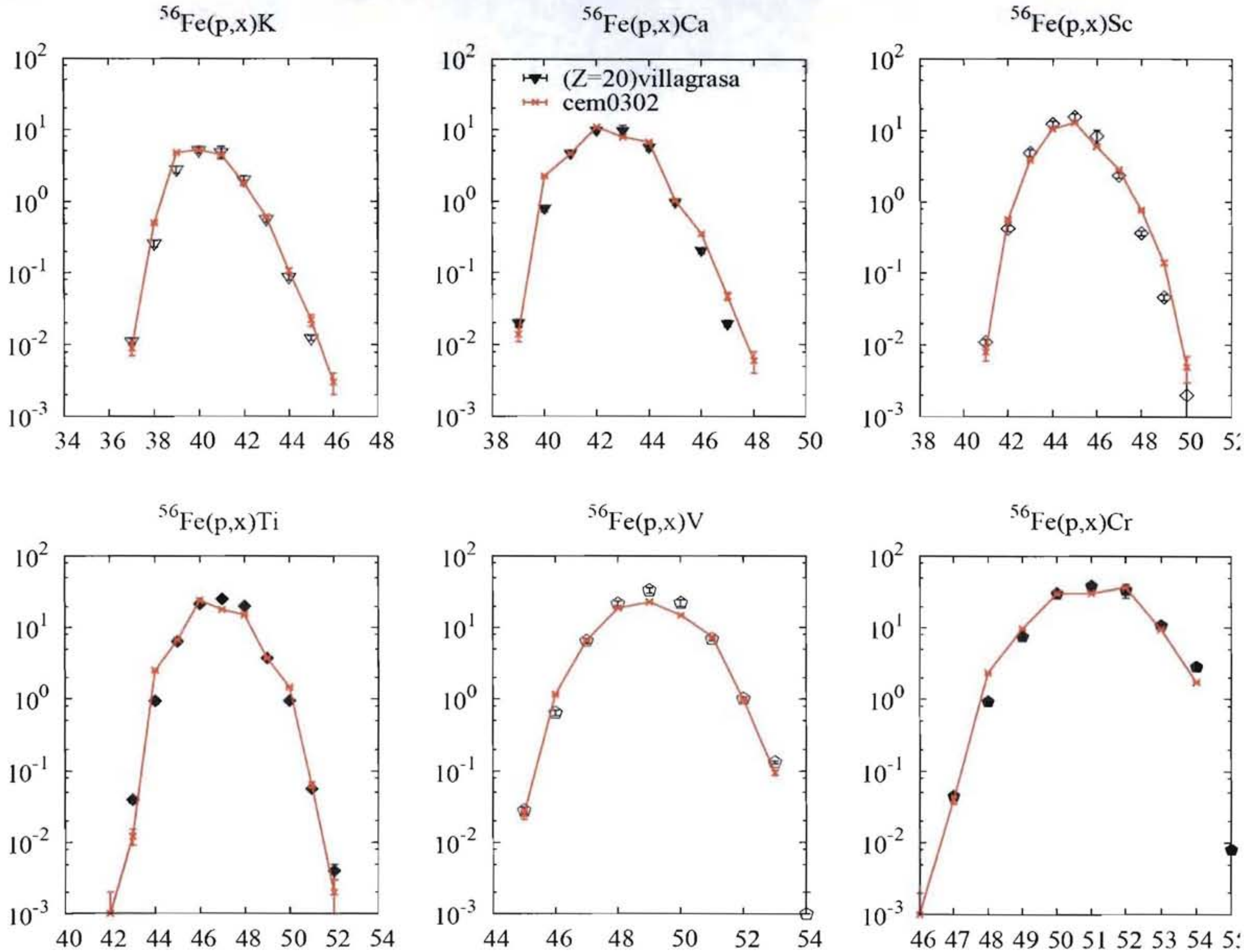


CEM03.02(.03) describes reasonably well the yield of fission fragments and spallation products from p + Pb and U, but underestimates production of light fragments with A ~ 25 from these reactions, just as most other models do

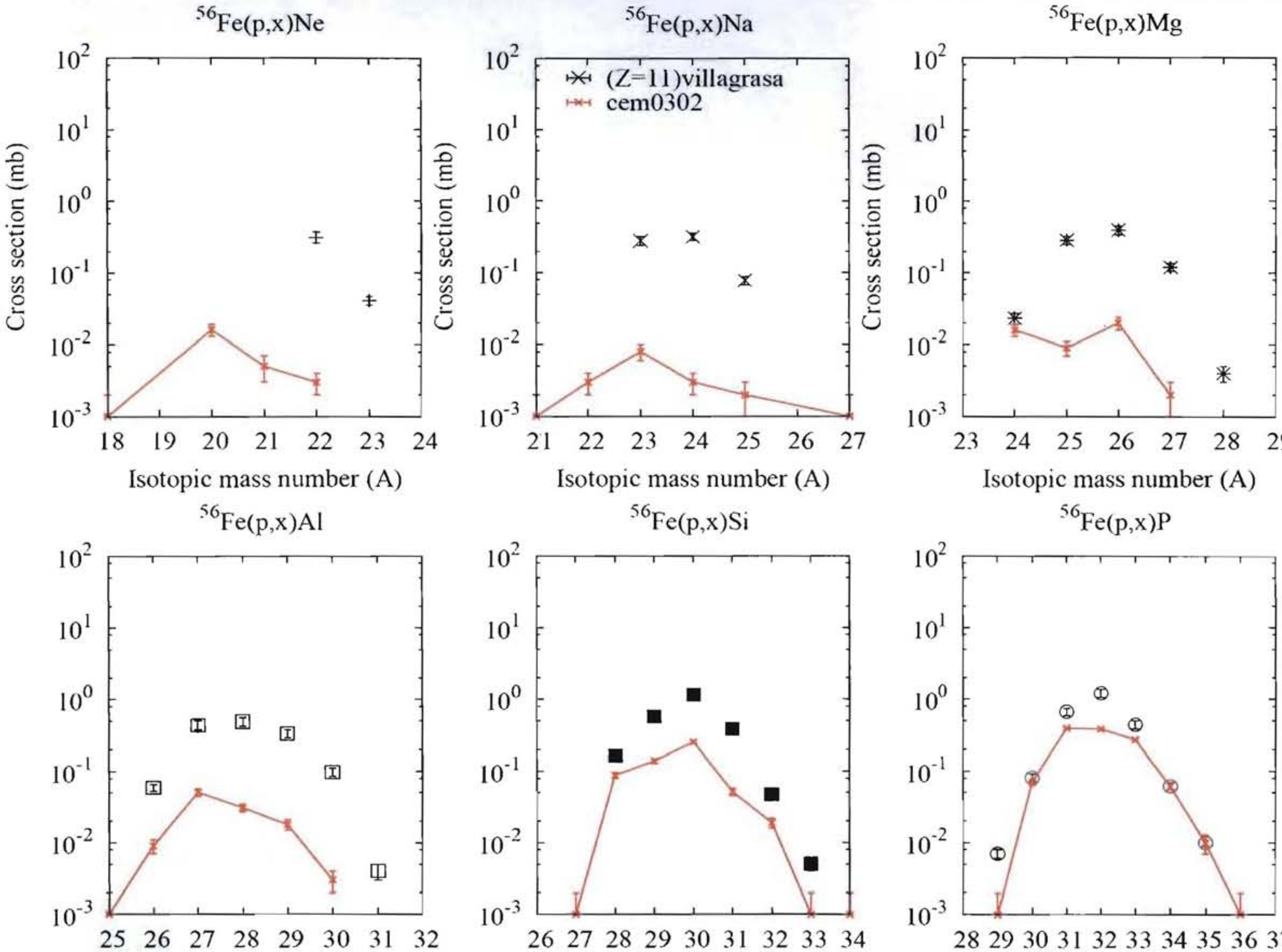




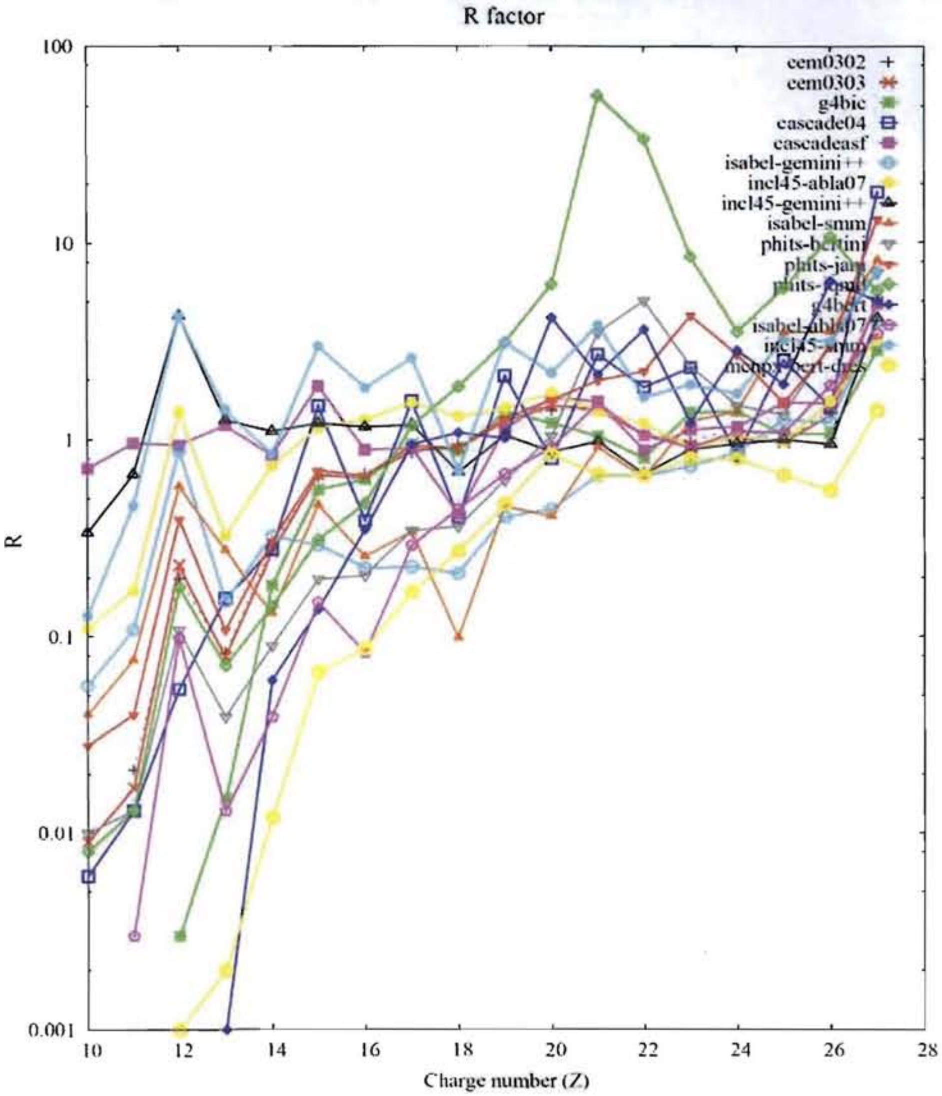
The agreement of CEM03.02(.03) charge distributions of fission fragments, spallation products, and light fragments with the measured data is very similar to the one observed above for the mass distributions

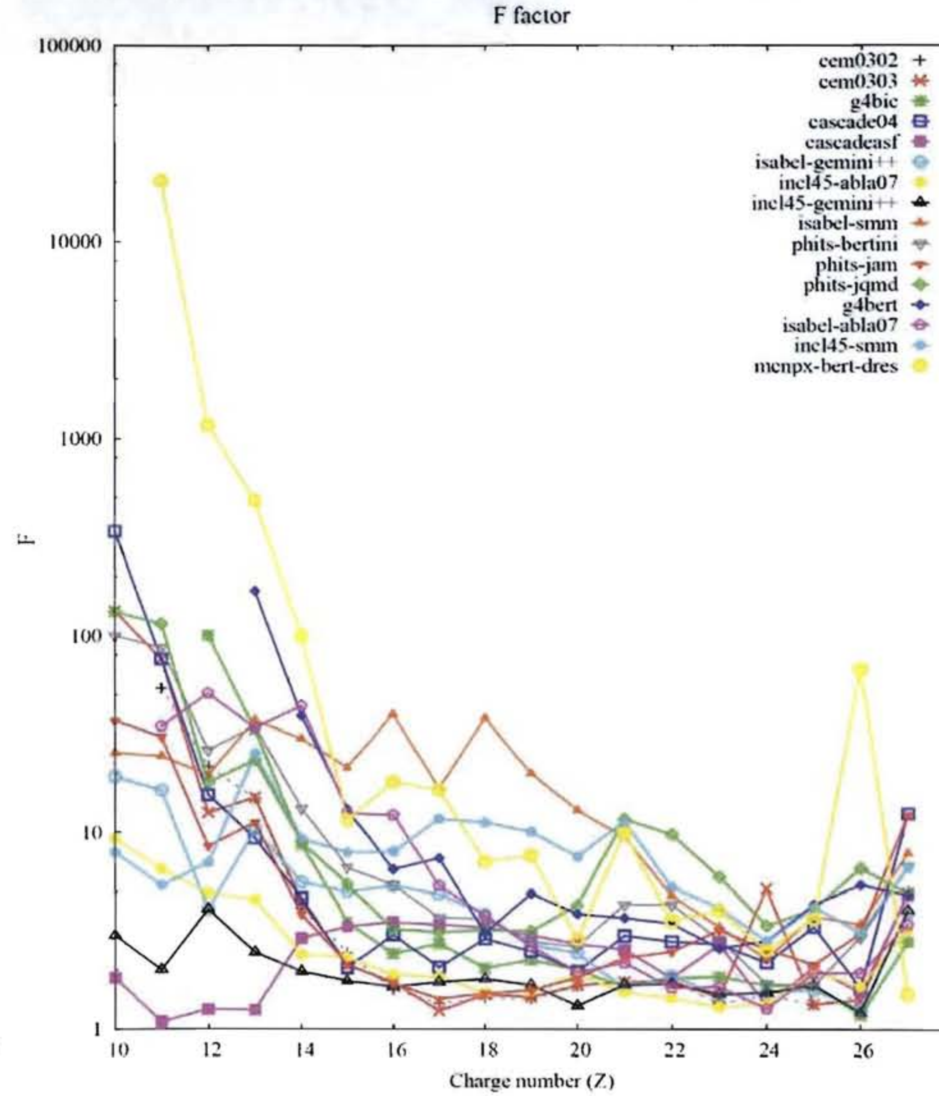


CEM03.02(.03) describes well the mass distributions of most individual not too light isotopes produced in the 300 MeV p + Fe reaction

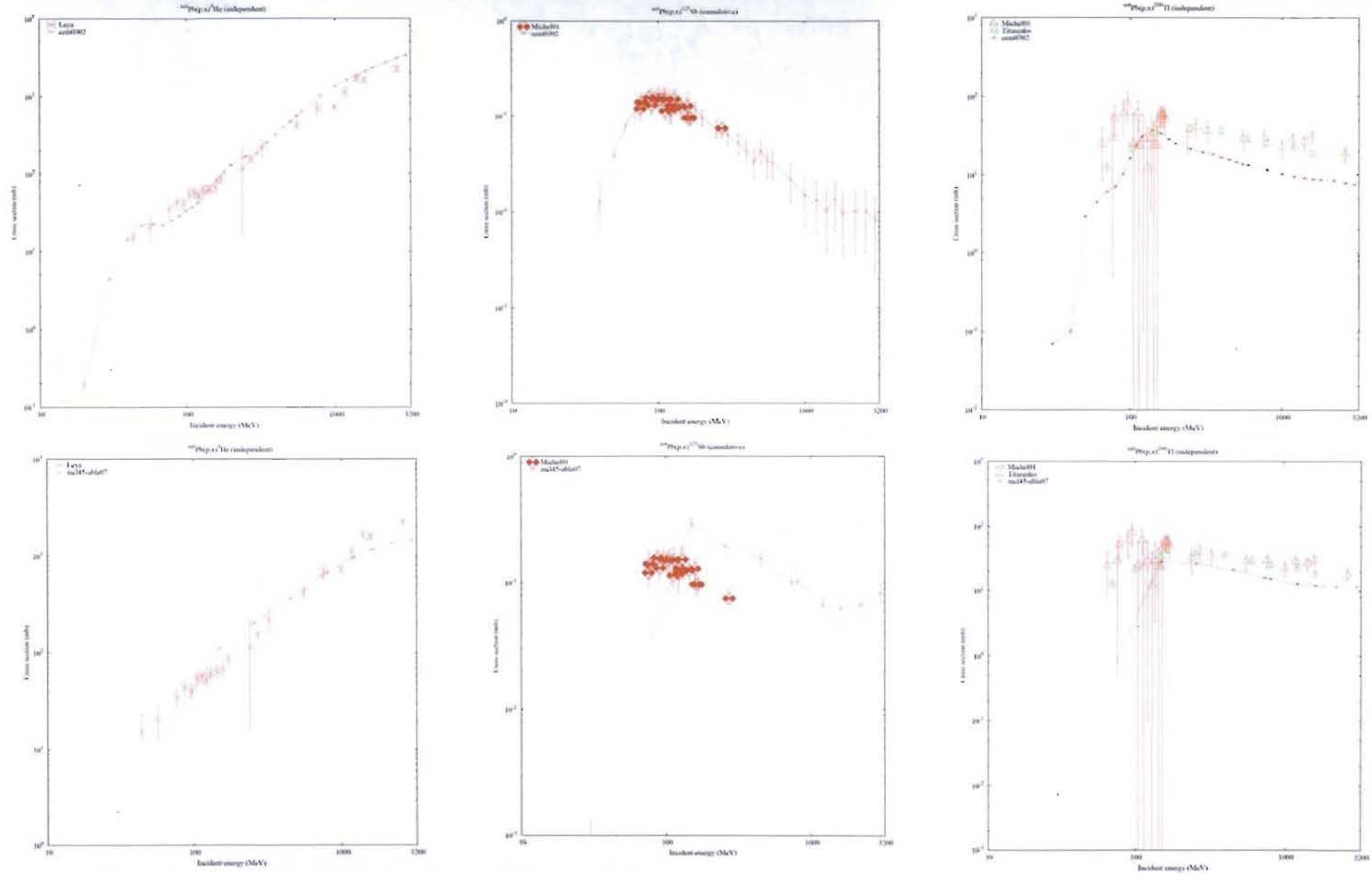


Yields of light Ne, Na, Mg, and Al isotopes produced in the 300 MeV p + Fe reaction are strongly underestimated by CEM03.02(.03), a serious problem still to be addressed also for most of other codes tested in our Benchmark, as shown by the figures of merit on the next viewgraph

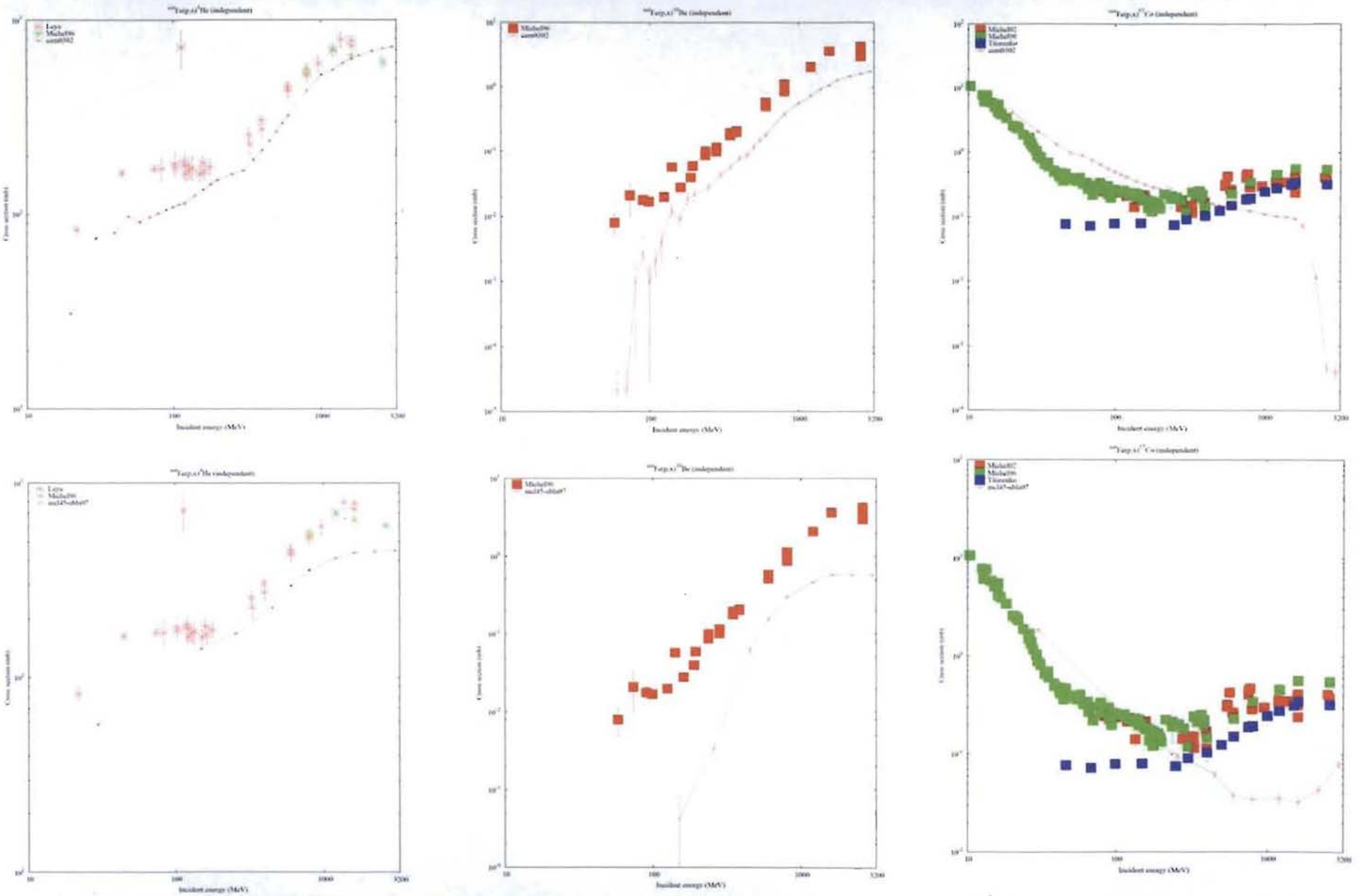




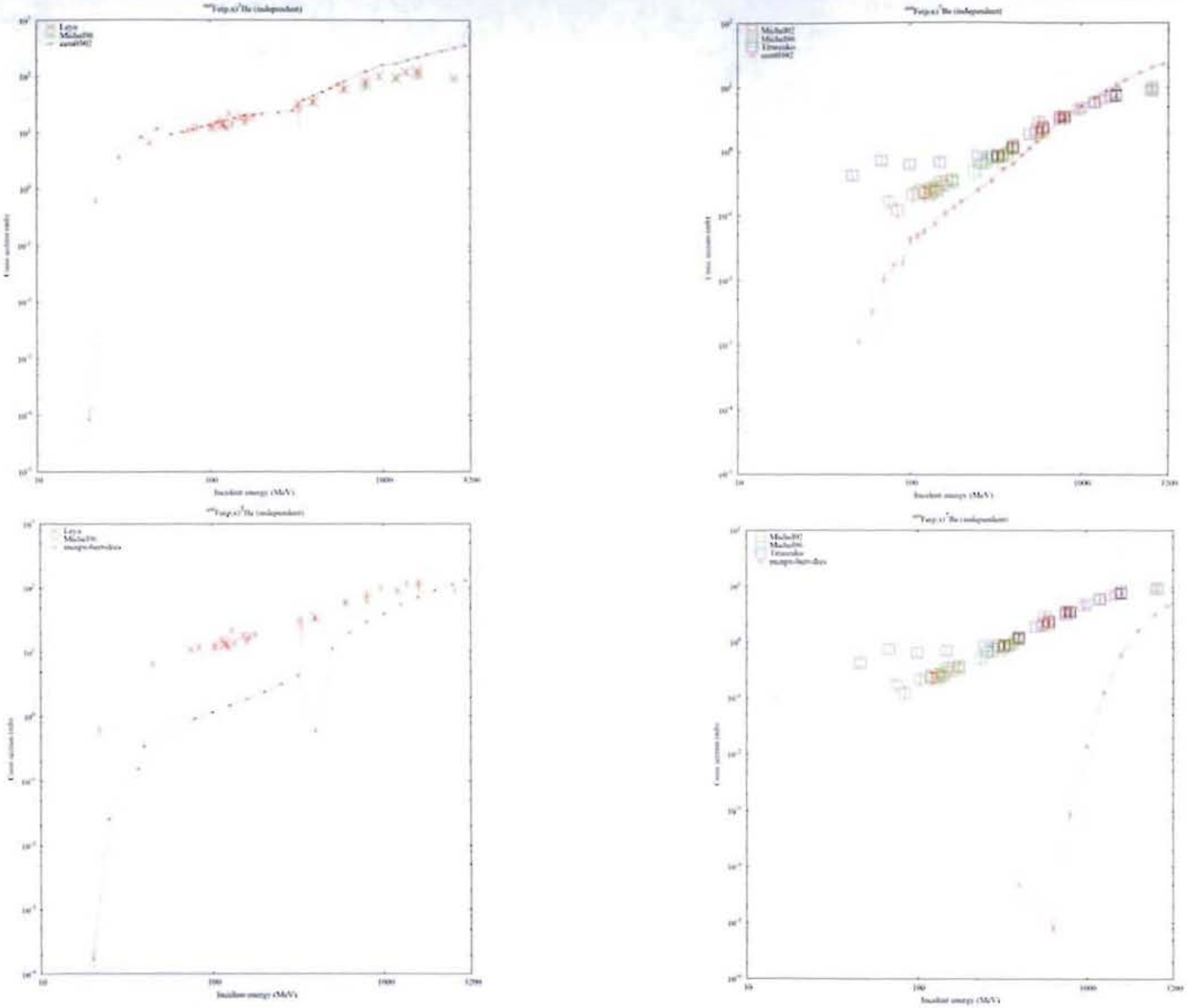
Both R and F deviation factors for isotopes produced in the 300 MeV p + Fe reaction vary significantly from the desired value of one with decreasing mass number of products and reach values of up to several orders of magnitudes for many of the codes



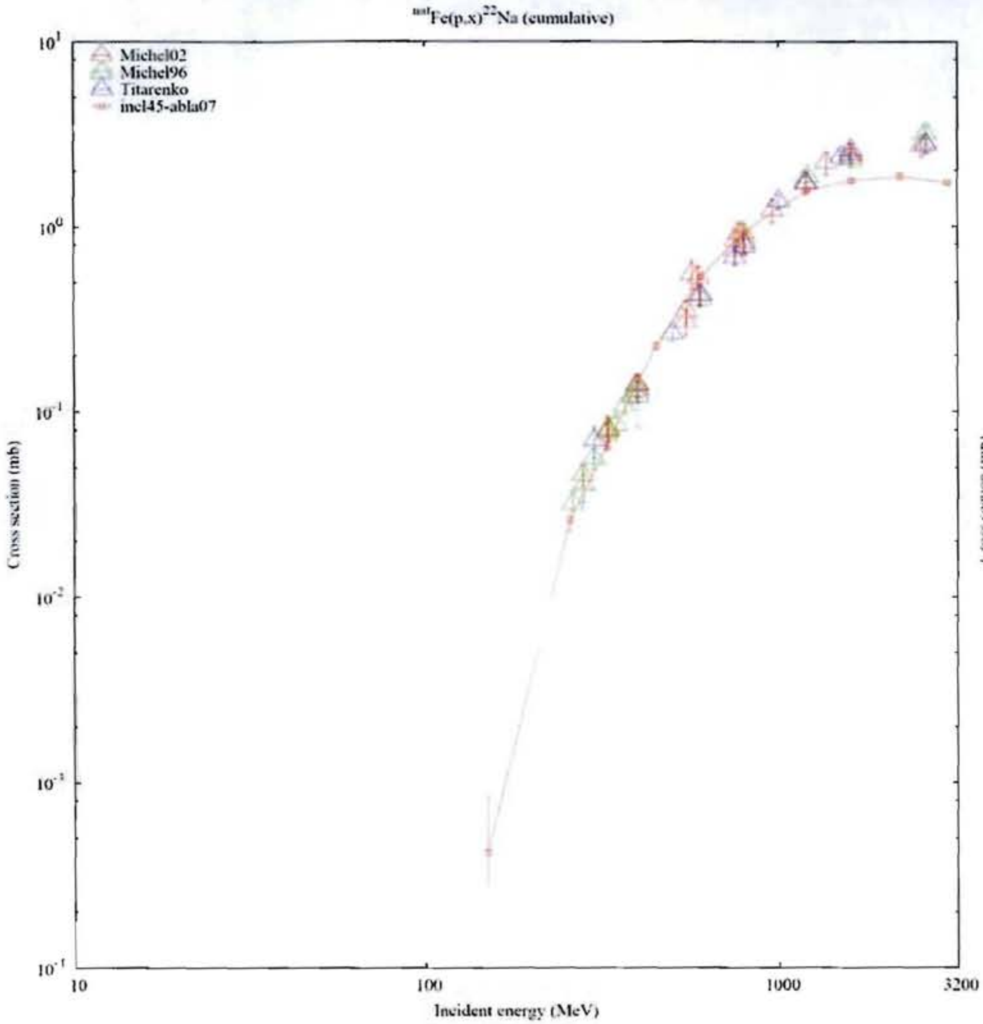
Excitation functions are the most difficult characteristics to predict; CEM03 often works well, but still has some problems

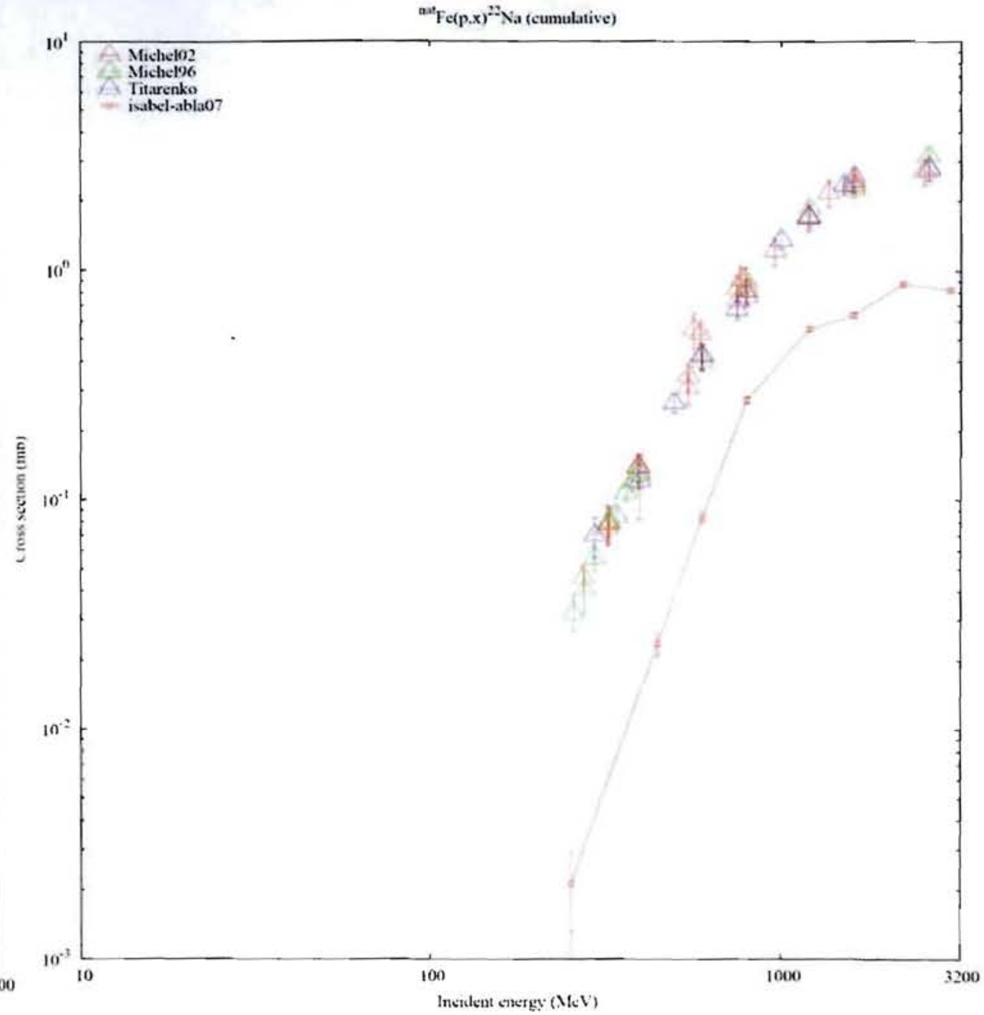


More examples of success and deficiency of CEM03.02 in describing several excitation functions for p + ^{nat}Fe reactions

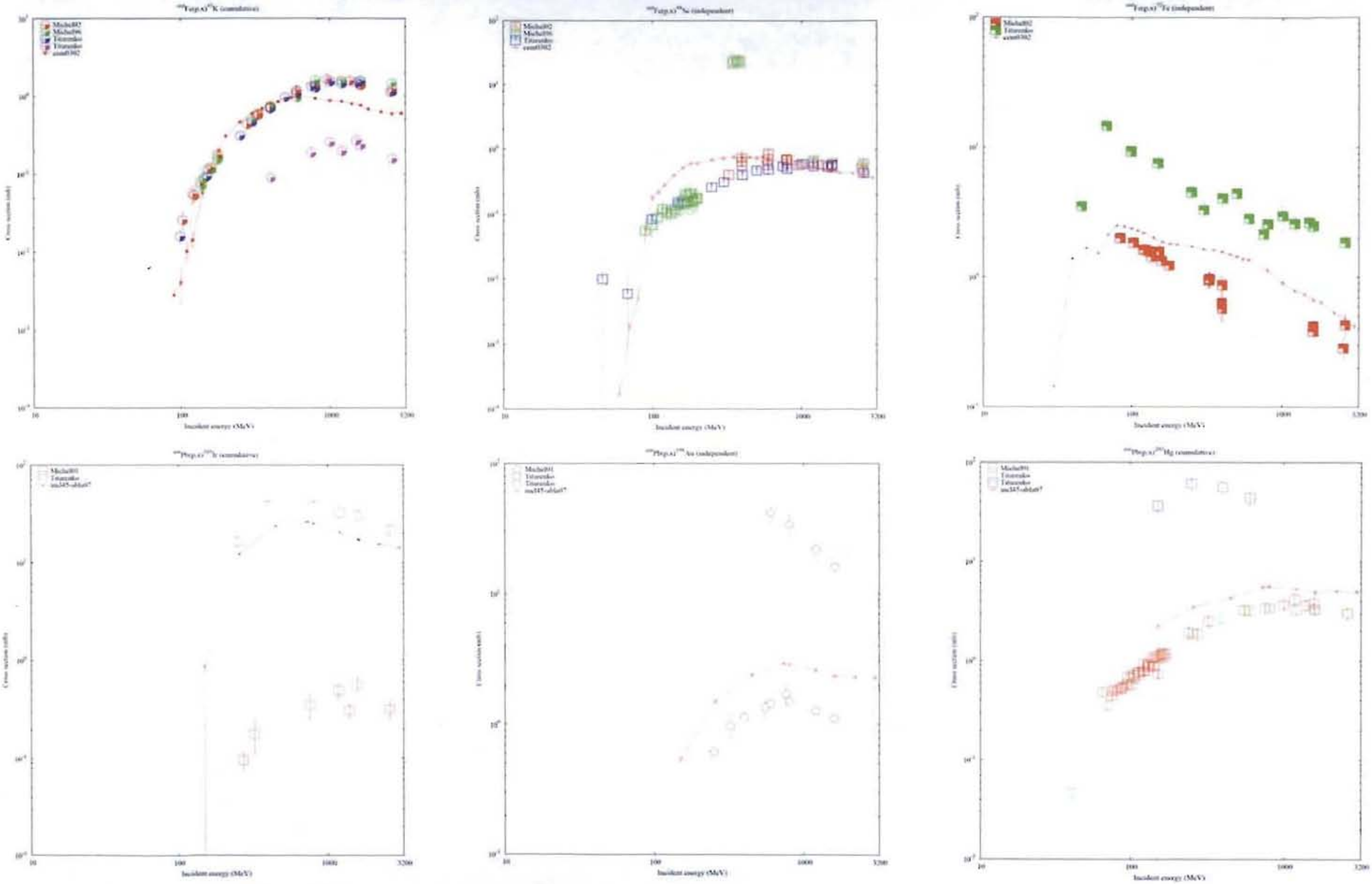


Examples of improved predictive power of MCNP6(X) for the production of ^{3}He and ^{7}Be from p + Fe reactions while using our CEM03.02 event generator in comparison with using the "default" Bertini INC + Dresner evaporation option





It is important to know that modules are "tuned" to each other while merging them into a single code, an idea adopted by CEM03.02(.03), LAQGSM, FLUKA, SHIELD, etc., but not understood or neglected by MCNPX, GEANT4, ALICE, CEM95, ...



We need reliable experimental data in order to develop better models and codes

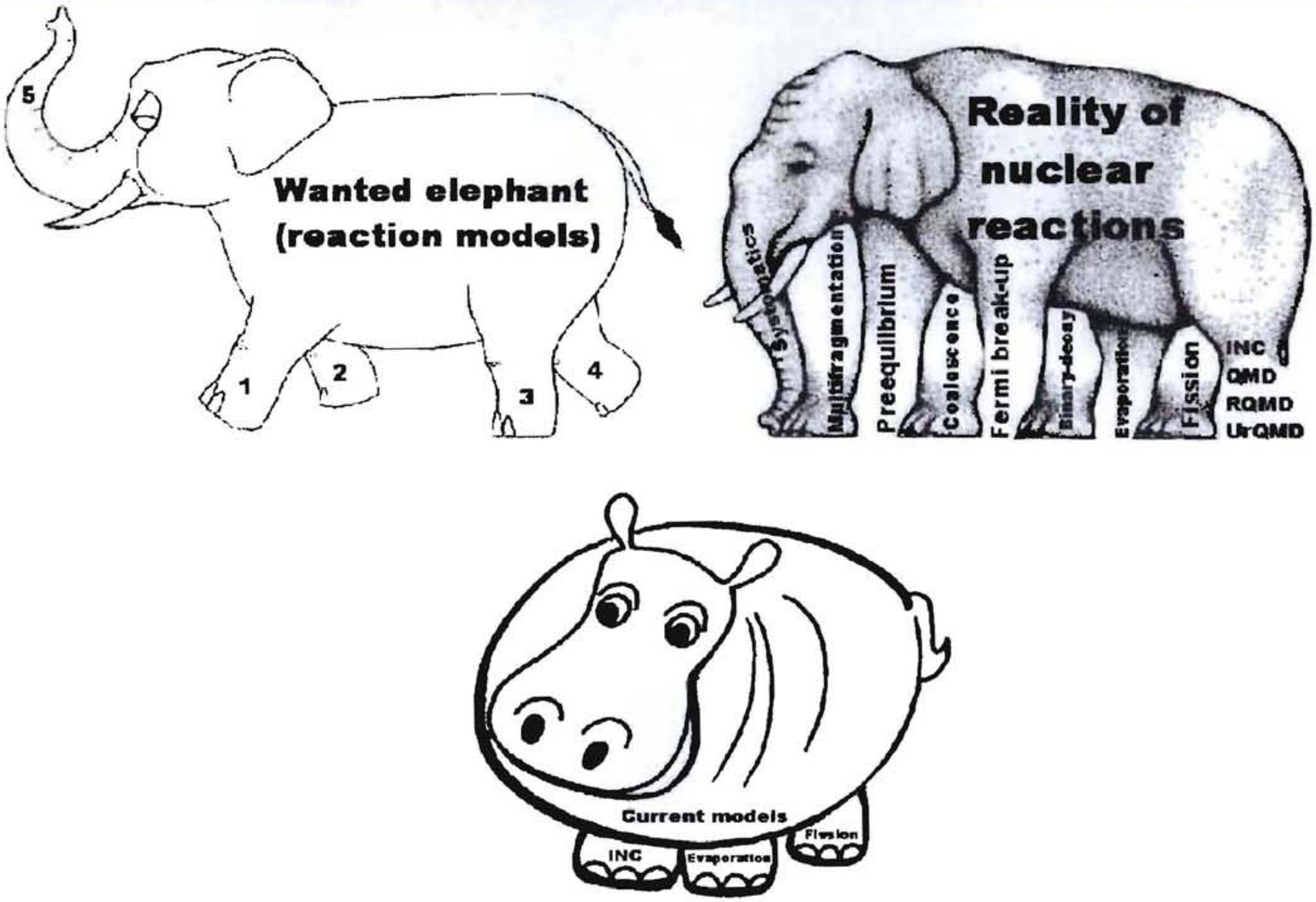


Fig. 10. The mathematical genius and one of the pioneers of the computer science and Monte Carlo particle transport, John von Neumann, used to say: *With four parameters I can fit an elephant, and with five I can make him wiggle his trunk* (the left elephant here). The reality for intermediate- and high-energy nuclear reactions is much more complicated; we can describe many features of such reactions considering only the INC, preequilibrium, evaporation, and fission models, each of them with tens of their own parameters (getting four legs for the right elephant). To describe complex particle and fragment emission from some reactions, we may need to consider other reaction mechanisms, like Fermi break-up, coalescence, multifragmentation, and fission-like binary-decays as described by the code GEMINI of Charity (getting now also four, but different, legs for the right elephant). Unfortunately, only by using systematics based on available experimental data may we describe well some characteristics (i.e., to make the right elephant wiggle his trunk). Some features of specific reactions are not described well by any current models; this is why the right elephant is still without a tail and with an unfinished leg. Establishing the real mechanisms of nuclear reactions and their contributions to specific measurable characteristics is like counting the legs of the right elephant; we can see four, five, or even eight legs, depending on our point of view. Some current nuclear reaction models try to describe all processes considering only INC, evaporation, and fission. In this case, we get only a hippopotamus, precariously balanced on three imperfect legs (lower plot).

Summary (1)

- CEM03.02(.03) describes reasonably well most of the tested reactions, therefore it can be employed with confidence as a reliable event generator in MCNP6 as the main "workhorse" for intermediate-energy applications.

- However, we have identified several problems to be solved to improve the predictive power of CEM03.02 (and CEM03.03), like: improvement of approximations used to describe nucleon and pion production in elementary interactions during the INC; considering preequilibrium emission (and maybe also coalescence production) of fragments heavier than ^{4}He; accounting for multifragmentation of highly excited nuclei and for "direct" knock out and pick-up processes of complex particle production, to name a few.

- One of the most important but difficult and time consuming improvements of CEM03.02(.03) would be development of a new and less phenomenological evaporation/fission model.

Summary (2)

- An important property of nuclear event simulation codes is how efficient they are. For large scale transport simulations, a speed factor of 5 to 10 can make a big difference. CEM03.02(03) is roughly this much faster than CEM95 for intermediate-mass nuclei.

- The Benchmark has proved once again that modules are "tuned" to each other while merging them into a single code: we can get bad results by combining arbitrary modules, as allowed currently by some transport codes.

- To understand the "real" mechanisms of nuclear reactions and develop better models, we need more measurements, including correlations.

We thank Drs. Sylvie Leray and Jean-Christophe David
for inviting us to present our CEM results
and for their kind help and cooperation !