Validation of Spallation Models

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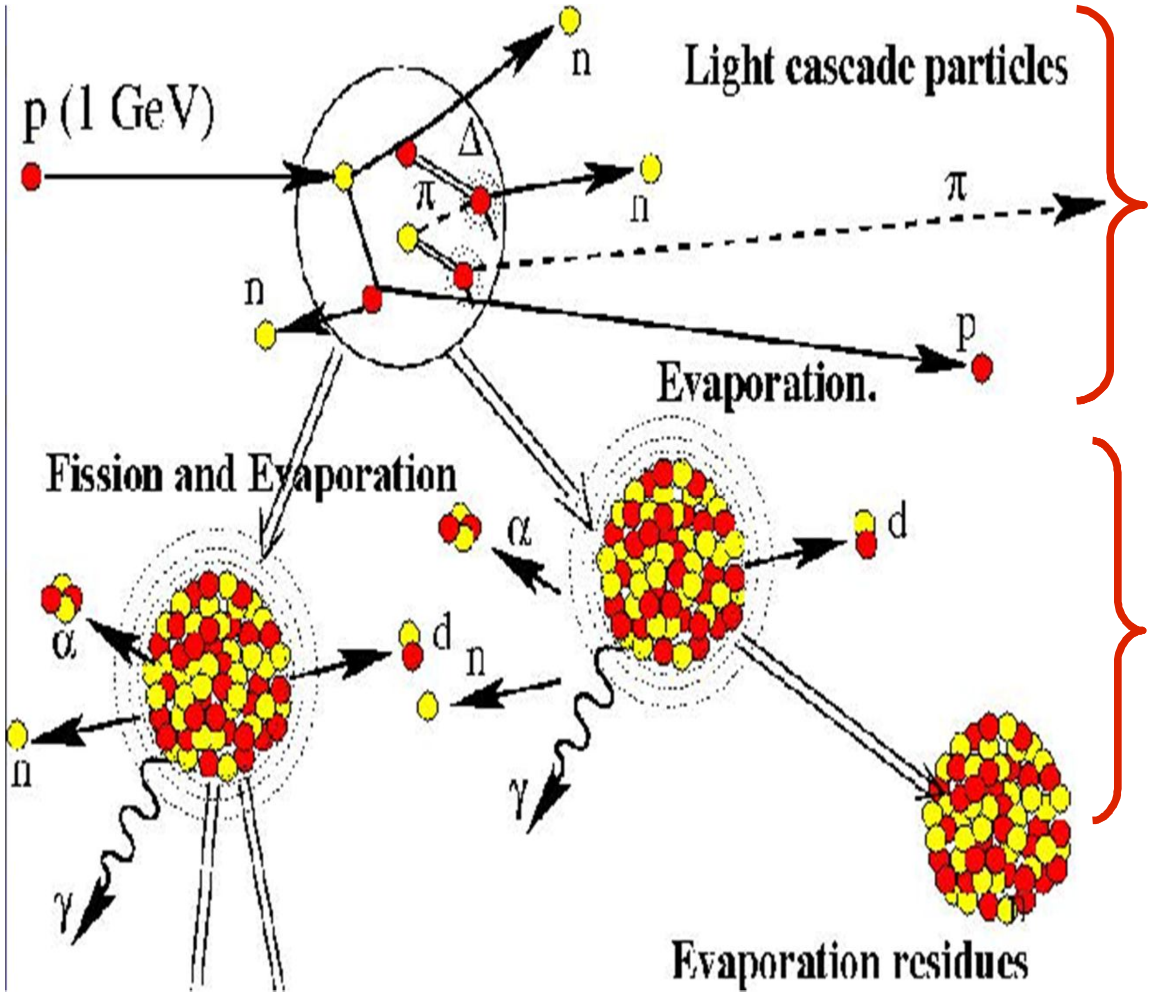
SPALLATION REACTIONS

Two Step Mechanism: R.Serber 1947



First Stage : NN, Nπ collisions
Fast process (≈ 30 fm/c)

Second Stage:
Slow process(≈ hundreds of fm/c)

PLAN OF INVESTIGATIONS

The task of the present investigations is to validate quality of data reproduction by different theoretical models.

To achieve this goal we need :

1. To select the data for purpose of validation of selected models
2. To find quantitative tests of the agreement between data and models
3. To choose one among available tests existing in the literature
4. To determine method of ranking of the models

EXP. DATA SET AND MODEL USED

Experimental data

Projectile Energy(MeV):

- 1200
- 2500

Protons →

Targets:

Symbol	A
1) Al	(27)
2) Au	(197)

Theoretical Models

INCL46 (Liege Intra Nuclear Cascade model) } First stage of reaction

SMM (Statistical Multi-fragmentation Model)

ABLA07

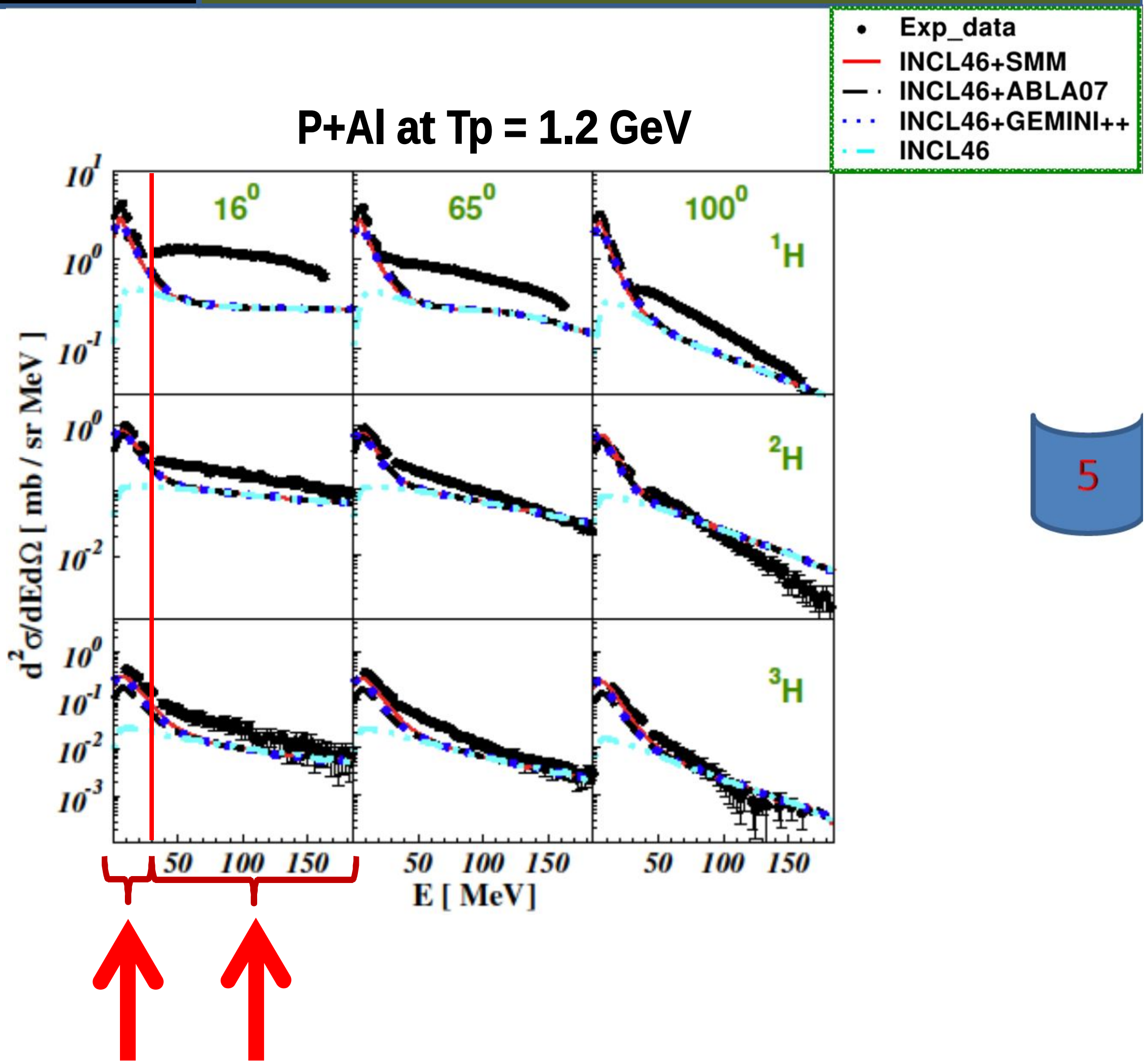
GEMINI++

} Second stage of reaction

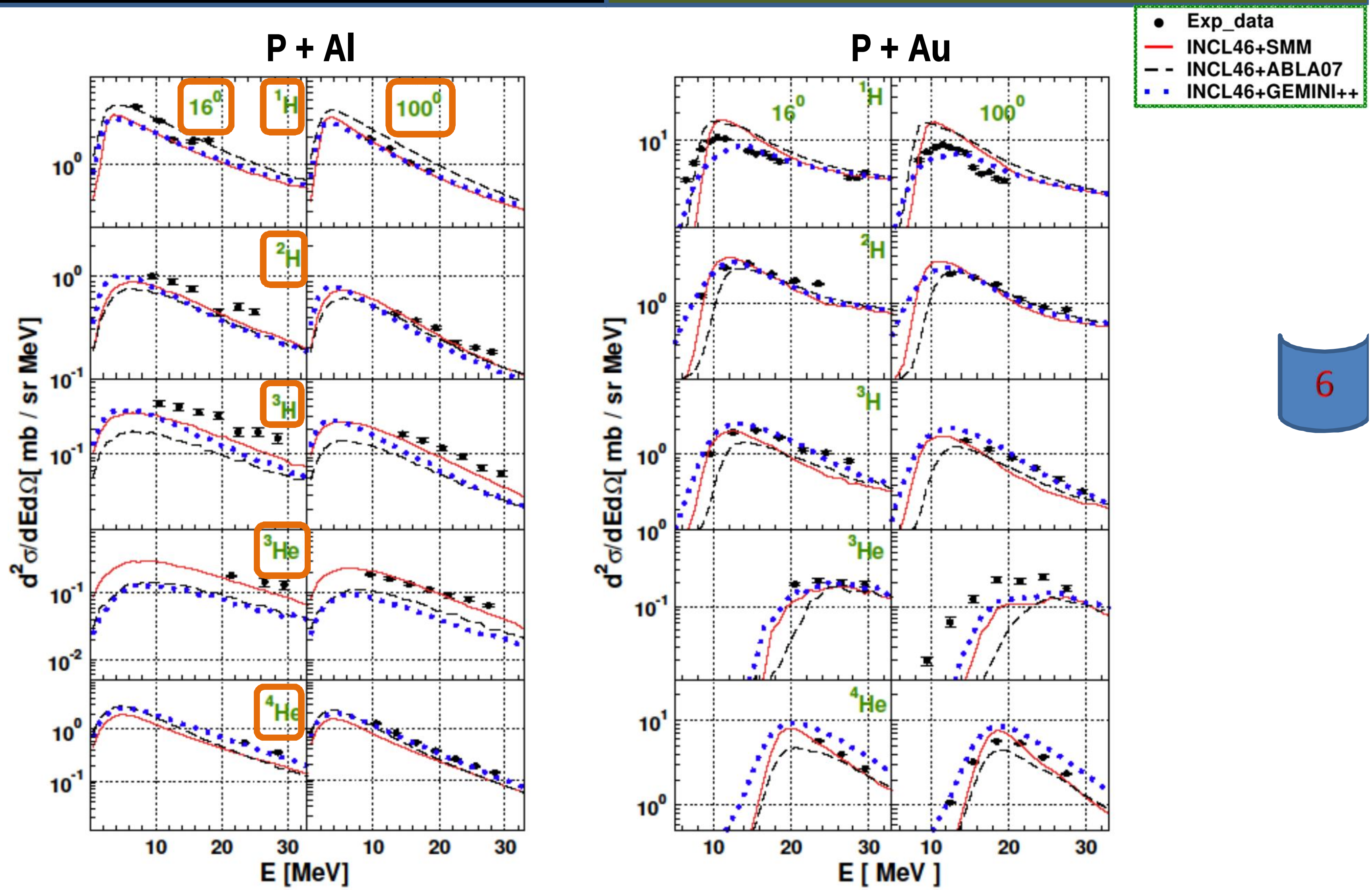
STRATEGY OF INVESTIGATIONS

Quality of data description by different models:

- Light blue lines show contribution from fast stage of reaction calculated by INCL4.6.
- Other lines show **sum** of this contribution and that from the second stage of the reaction calculated by 3 different models: **SMM**, **ABLA07**, and **GEMINI++**.
- It is evident that contribution of latter processes is significant only at low energies.
- Therefore the judgment of the agreement between models and the experimental data will be done separately for **E_{ejec} <= 30 MeV**
- and for **E_{ejec} > 30 MeV**



Tp = 1.2 GeV (E <= 30 MeV)



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Remarks

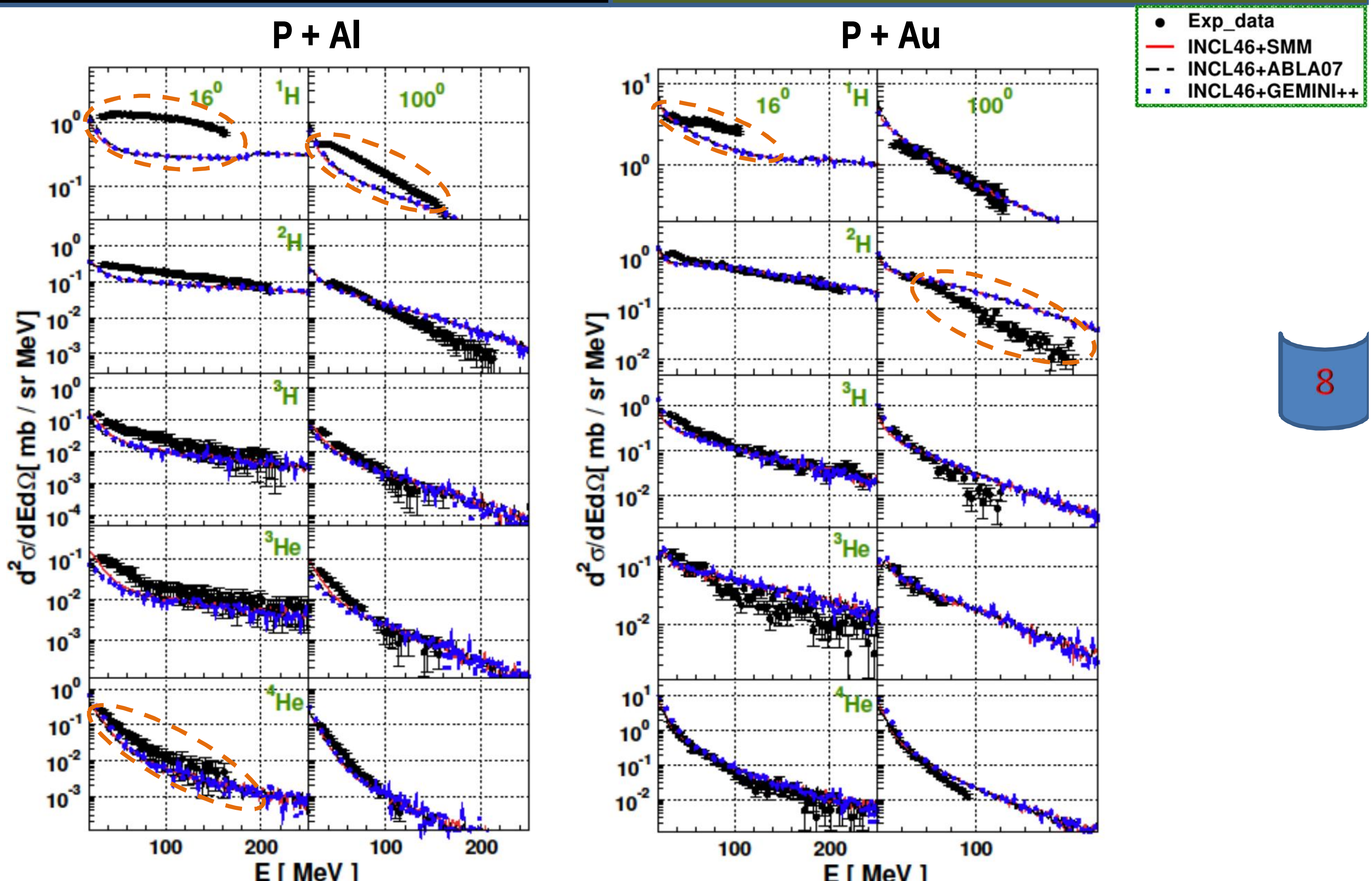
- In the previous slide, significant differences between predictions of various models were visible because the low energy spectra may be populated by sequential evaporation of particles as well as by multifragmentation of excited remnants of the first stage of the reaction and different theoretical models describe these processes with **different approximations** using also **different parameters.**
- Two problems arise:

1) To decide whether the model description is satisfactory
2) Which of the models gives the best description

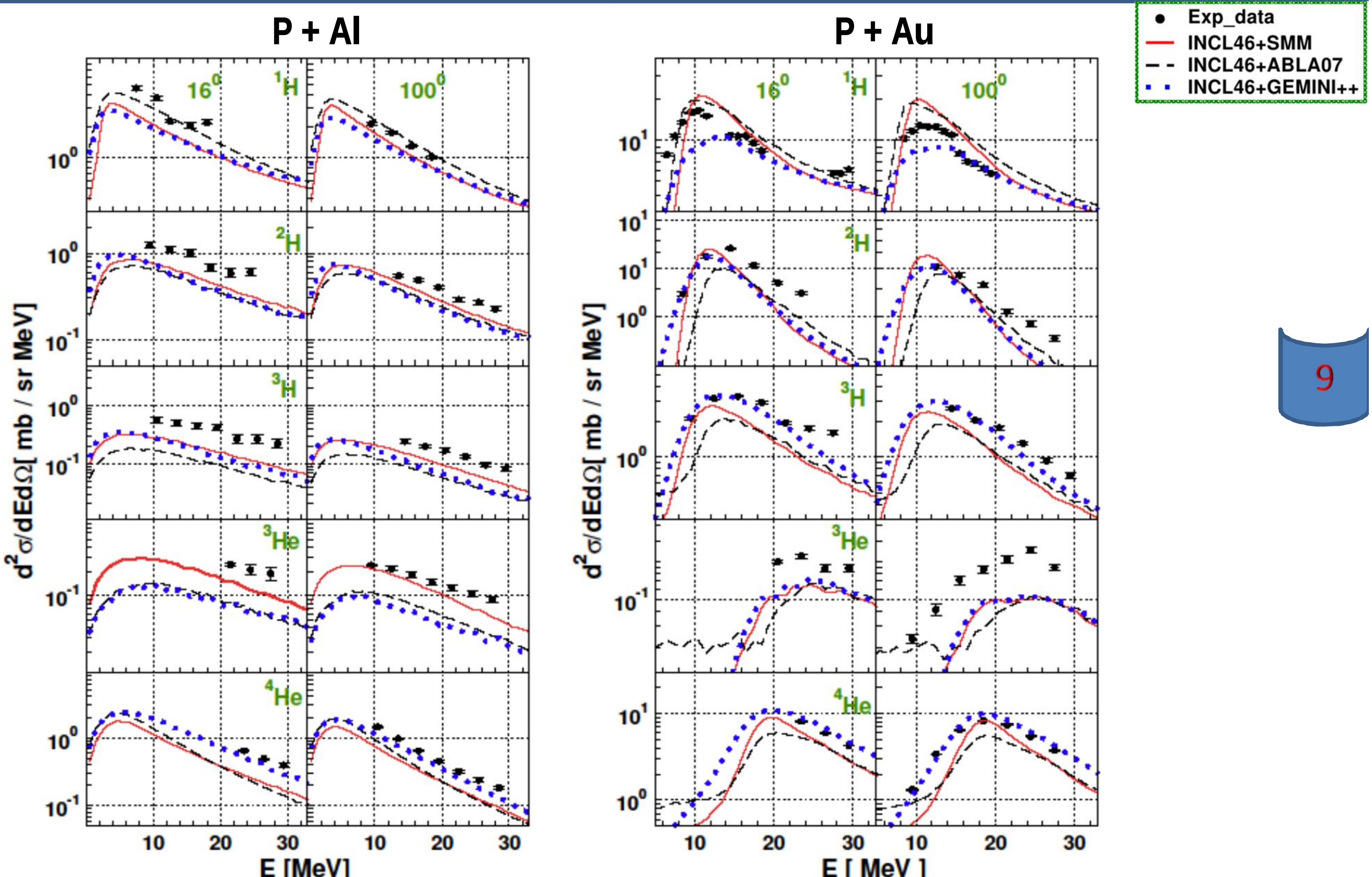
- **It is necessary to use quantitative measures (statistical tests) to solve these problems**.

- In the next slide the high energy region of the spectra is shown, where only fast reactions described by INCL4.6 . Therefore only the first of the above problems should be solved : to decide whether the model description is satisfactory **but it also needs the quantitative estimation of (dis)agreement of model and data cross sections.**

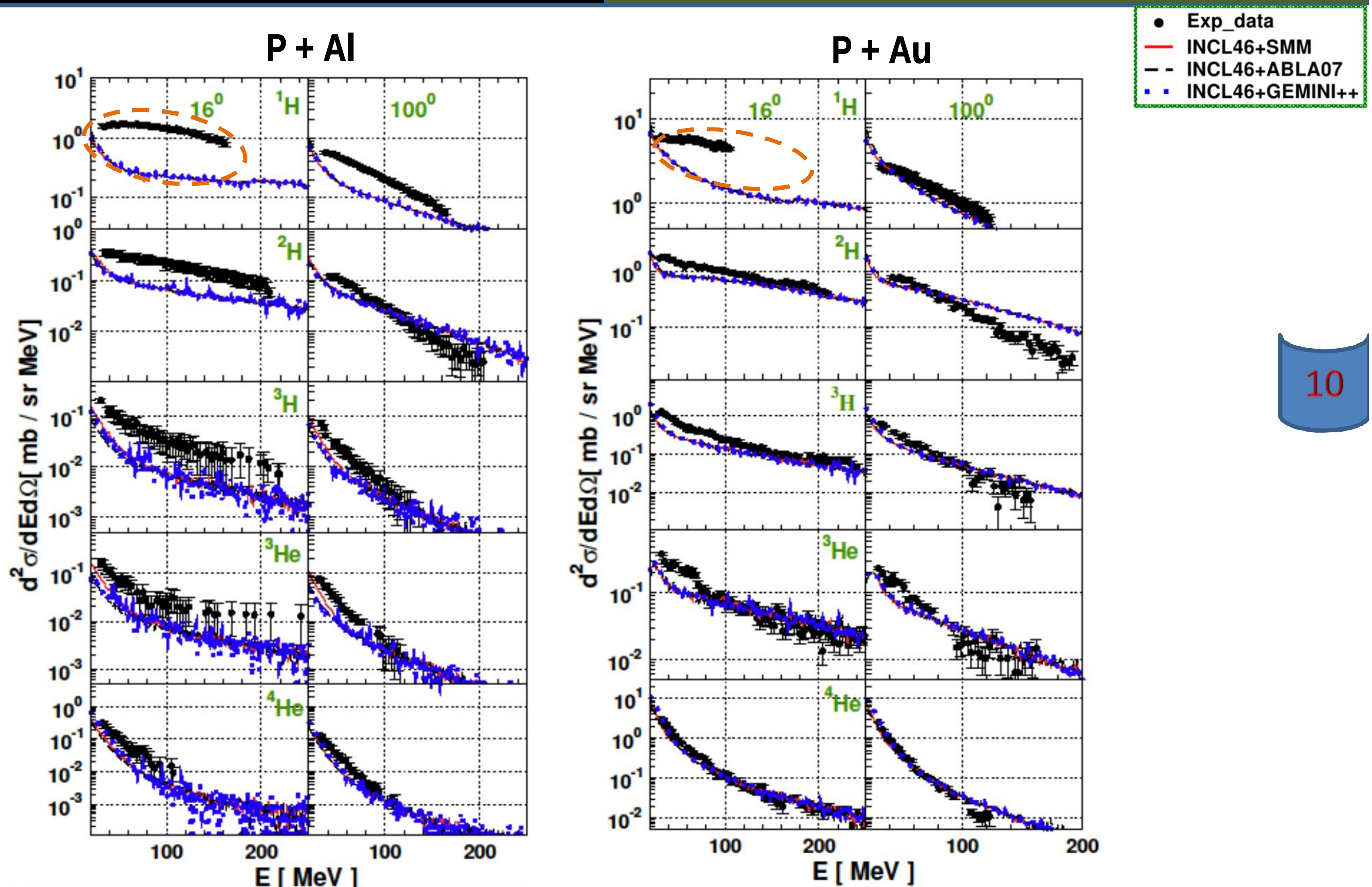
Tp = 1.2 GeV (E > 30 MeV)



Tp = 2.5 GeV (E <= 30 MeV)



Tp = 2.5 GeV (E > 30 MeV)



NEED FOR STATISTICAL FACTORS OR TESTS ?

- The **qualitative** differences between the data and model calculations allow to conclude about general aplicability of the models
- However, they do not allow to judge in **objective** manner about quality of different model descriptions i.e. they do not allow for the ranking of models.
- One has to use some **quantitative** measures of (dis)agreement of the data and theoretical cross sections.
- There are many **tests (statistics)** used in the literature for this purpose.

For each of them we should know

- **Expected value** of the test in case of ideal agreement
- **The spread of values** of the test around this expected value

Deviation factor (ε)

- It is proposed to use as a measure of the quality of the model **the deviation test – "ε (test)"** of given statistical **test** from its expectation value **E(test)** obtained in the case of **perfect agreement** between the model and experimental cross sections.
- This deviation is normalized to the standard deviation σ_{stat} of the test which always appears because of **statistical errors of the data**.

$$\varepsilon(test) = \frac{test - E(test)}{\sigma_{stat}(test)}$$

Where test = H , D , R , F , L

H - Test

1. Mean weighted deviation or H factor (similar to chi-square)
[N.V. Kurenkov et al., ARI 50 (1999) 541]

$$H = \left(\frac{1}{N} \sum_{i=1}^{N} \left(\frac{\sigma_i^{exp} - \sigma_i^{calc}}{\Delta \sigma_i^{exp}} \right)^2 \right)^{1/2}$$

The H test is unique in this sense that for the perfect agreement of the model cross sections with the experimental data **its probability distribution function** and therefore the expectation values E(H) and the standard deviation σ(H) **may be found analytically** providing that the following, commonly used assumptions are fulfilled:

- **The experimental data are independent Gaussian variables with Standard deviation equal to statistical error of data.**
- **Expectation value of the cross section equal to the measured cross section**

These formulae are presented in the next slide as functions of the number of experimental points N

Analytically derived parameters for H - Test

Probability density function of the test H (N is number of the cross sections)

$$h(H) = \frac{N^{N/2}}{2^{N/2-1}\Gamma(N/2)} \exp\left(-\frac{NH^2}{2}\right) \cdot H^{N-1}$$

Expectation value E(H) and **variance var(H)** of the test H

$$E(H) = \sqrt{\frac{2}{N}} \cdot \frac{\Gamma\left(\frac{N+1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}$$

$$var(H) = 1 - E(H)^2$$

Remarks

For tests used in the literature (different from H-test) this information is not known.

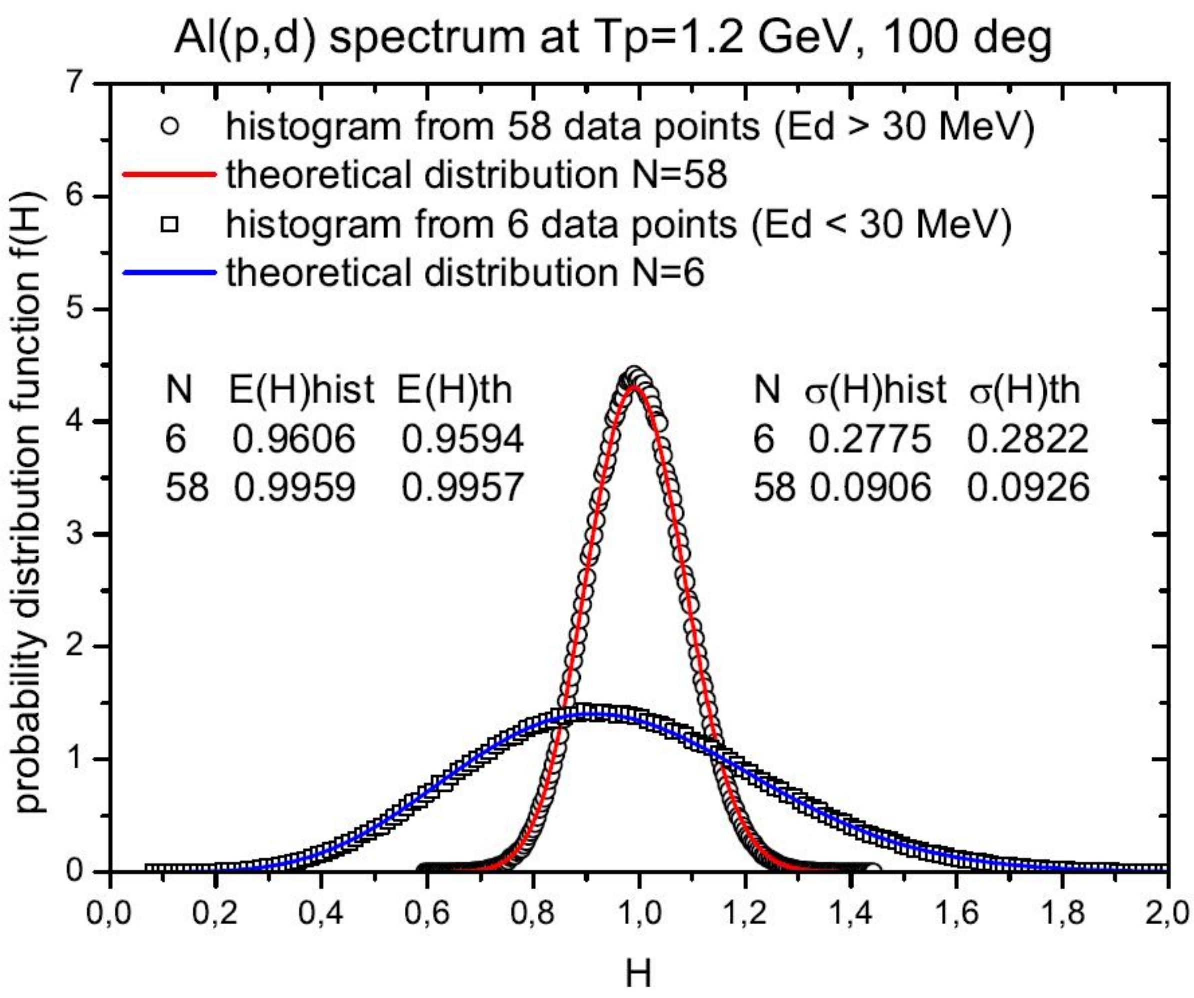
Therefore we propose to generate the probability distributions of various tests by Monte Carlo method performing sampling of the „data"

- according to Gaussian distributions with the expectation values of the data equal to actually measured cross sections
- the standard deviations equal to statistical errors of the experimental data.

The H test may be used to check whether such a sampling leads to the same result as analytically calculated probability distribution functions and their parameters: E(H) and σ(H).

Comparison of histograms generated for H-test according to the above prescription with the exact probability distribution functions is shown in the next slide.

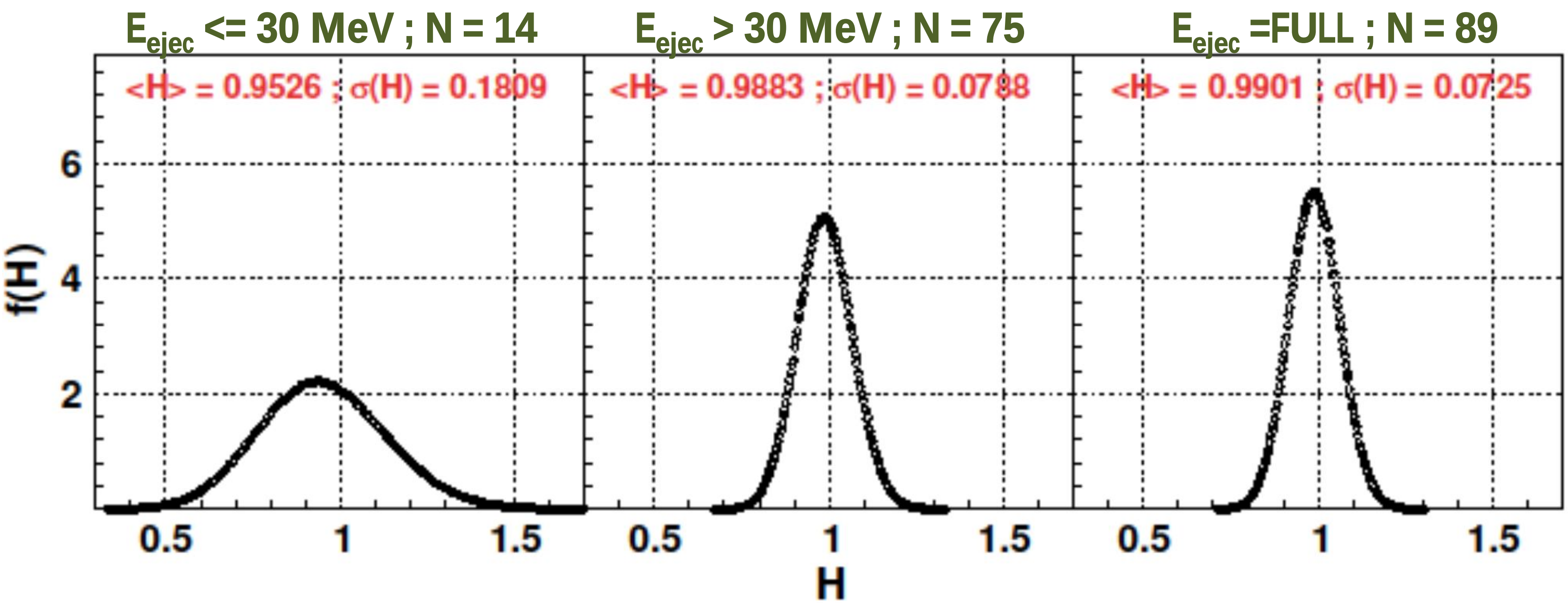
Comparison


Al(p,d) spectrum at Tp=1.2 GeV, 100 deg
histogram from 58 data points (Ed > 30 MeV)
theoretical distribution N=58
histogram from 6 data points (Ed < 30 MeV)
theoretical distribution N=6
N E(H)hist E(H)th
6 0.9606 0.9594
58 0.9959 0.9957
N σ(H)hist σ(H)th
6 0.2775 0.2822
58 0.0906 0.0926
probability distribution function f(H)
H
0,0 0,2 0,4 0,6 0,8 1,0 1,2 1,4 1,6 1,8 2,0
0 1 2 3 4 5 6 7

H Test

- **Expected Value (for Ideal agreement) ≈ 1**

Au(p,p) spectrum at 1.2 GeV , 16^0



Similarly, we did this for all the other tests with same exp data as used above:

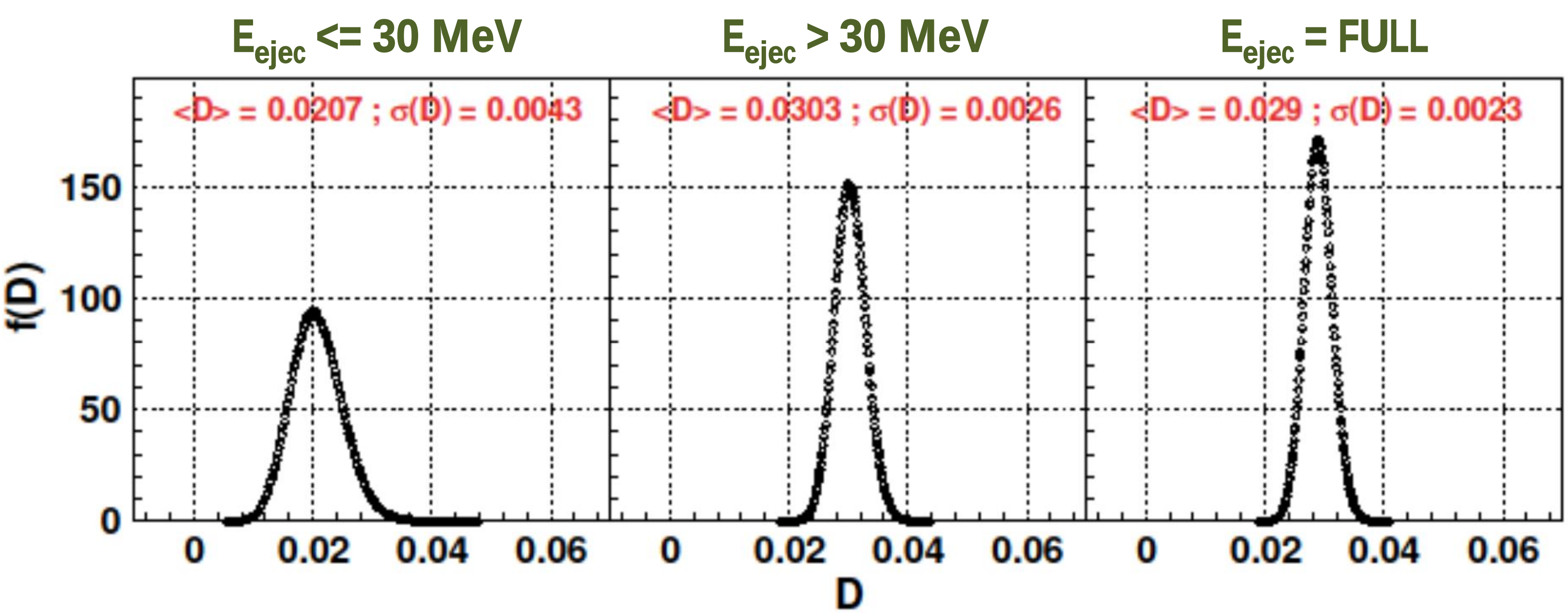
D Test

2. Relative variance of theoretical and experimental data

[N.V. Kurenkov et al., ARI 50 (1999) 541]

$$D = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{\sigma_i^{\exp} - \sigma_i^{calc}}{\sigma_i^{\exp}}\right|$$

- **Expected Value (for Ideal agreement) ≈ 0**

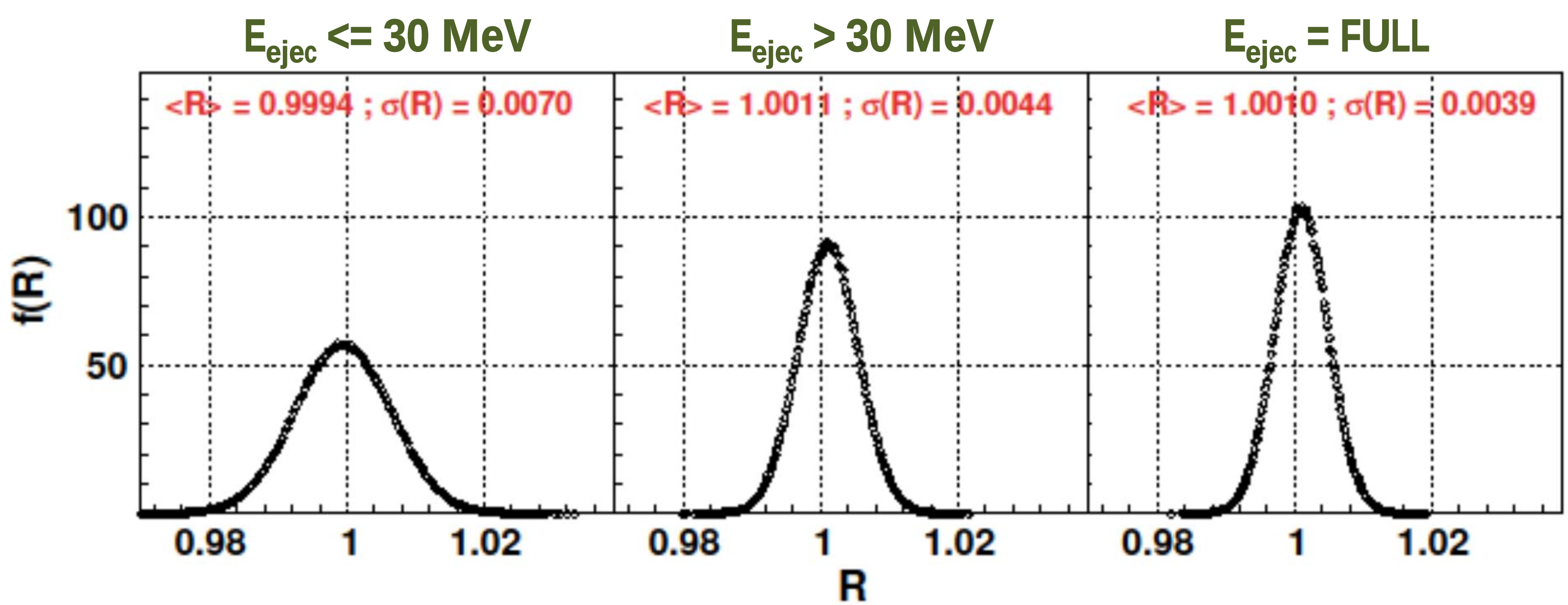


R Test

3. Ratio of calculated to experimental values
[C.H.M. Broeders et al., J. Nucl. Radiochem. Sci., 7 (2006) N1]

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

- **Expected Value (for Ideal agreement) ≈ 1**

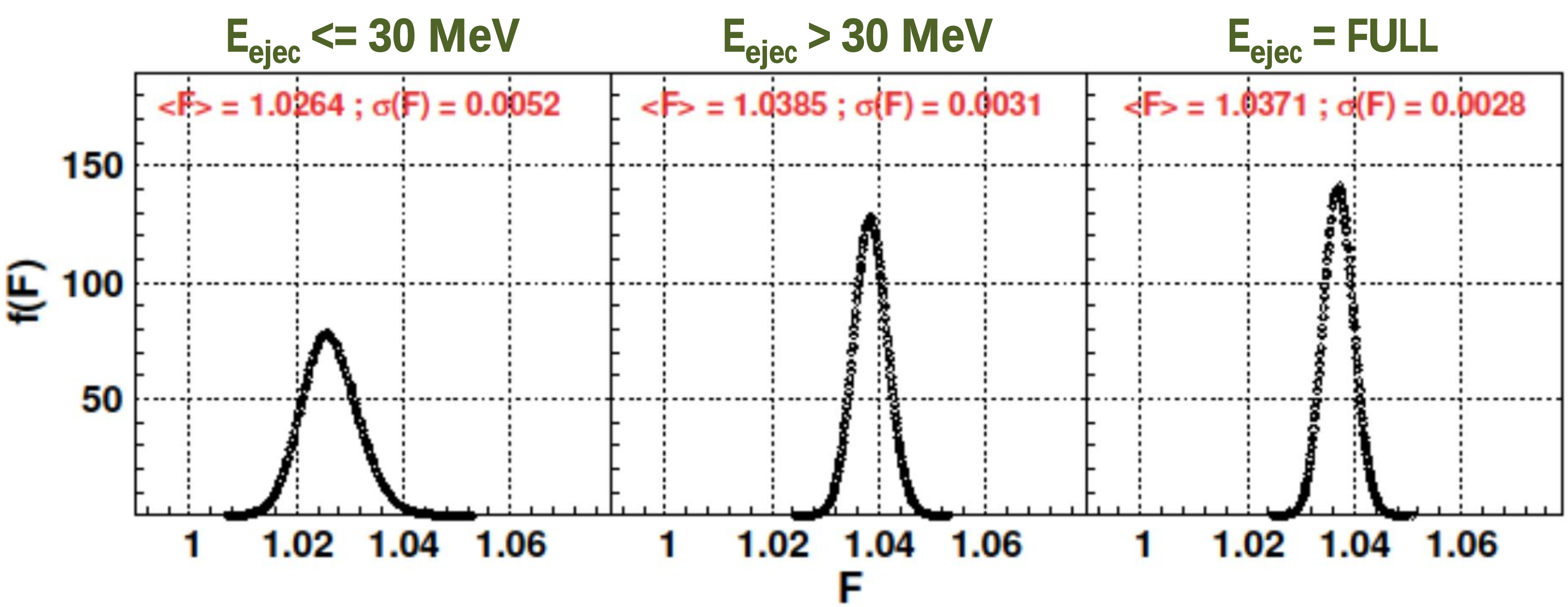


F Test

4. Mean square deviation factor
[Yu.E. Titarenko et al., PRC 78 (2008) 034615; R. Michel et al., NIMB 129 (1997) 53]

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

- **Expected Value (for Ideal agreement) ≈ 1**

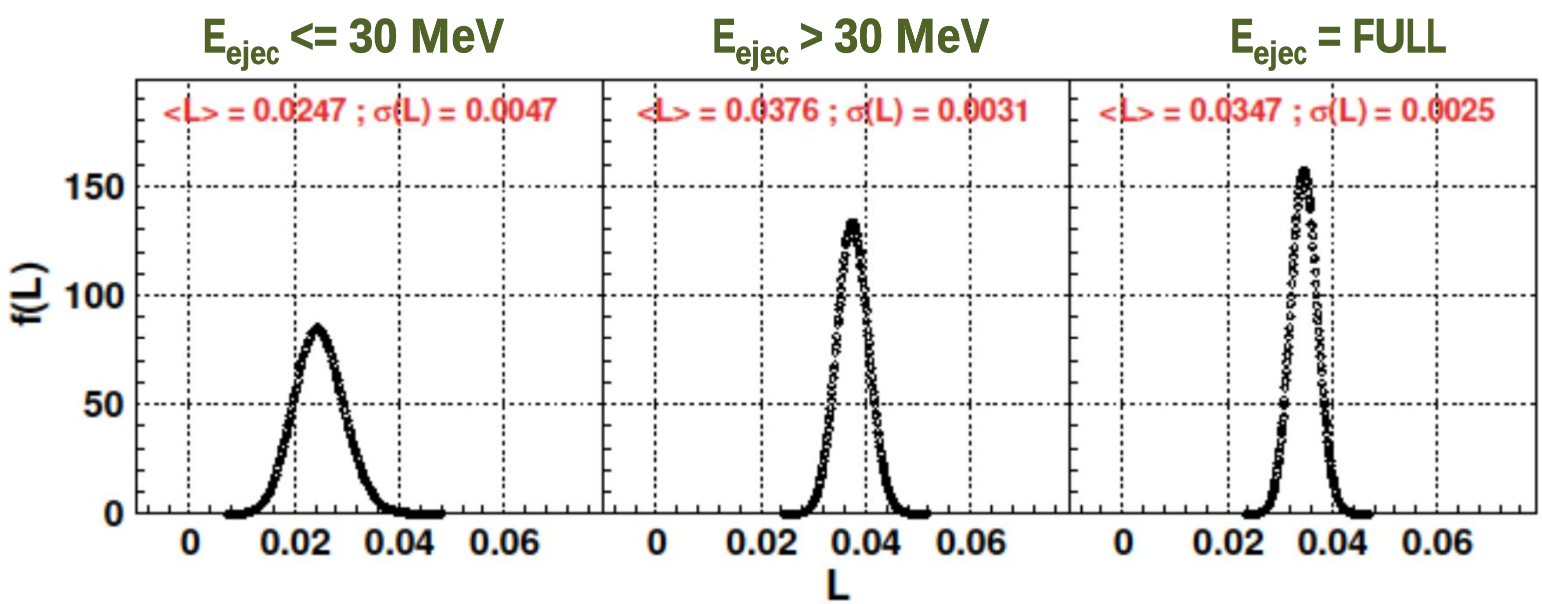


L Test

5. **Leeb factor** [H. Leeb et al., ND 2004, pp. 161]

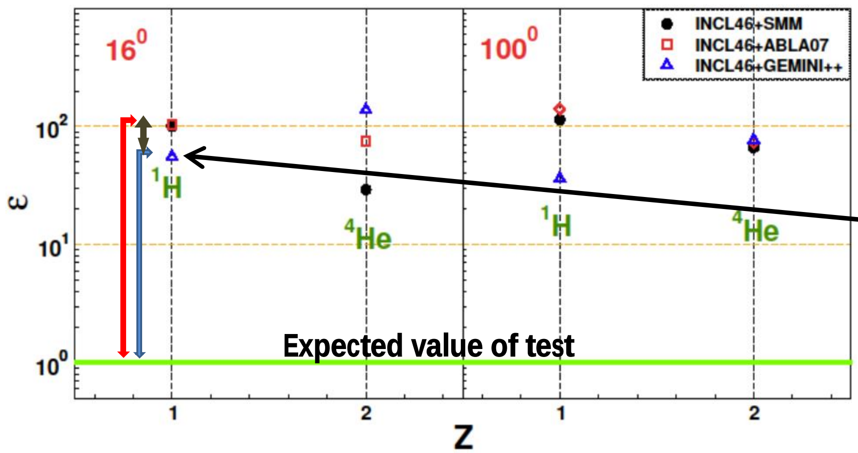
$$L = \left[\sum_{i=1}^{N} \left(\frac{\sigma_i^{calc}}{\Delta\sigma_i^{exp}} \right)^2 \left(\frac{\sigma_i^{calc} - \sigma_i^{exp}}{\sigma_i^{calc}} \right)^2 \Bigg/ \sum_{i=1}^{N} \left(\frac{\sigma_i^{calc}}{\Delta\sigma_i^{exp}} \right)^2 \right]^{1/2}$$

- **Expected Value (for Ideal agreement) ≈ 0**

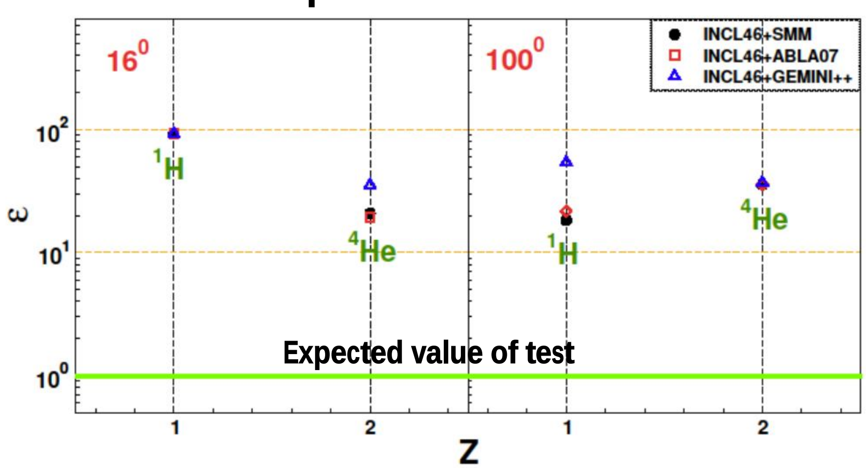


EXAMPLE FOR H-TEST for P + AU at T_P = 1.2 GeV

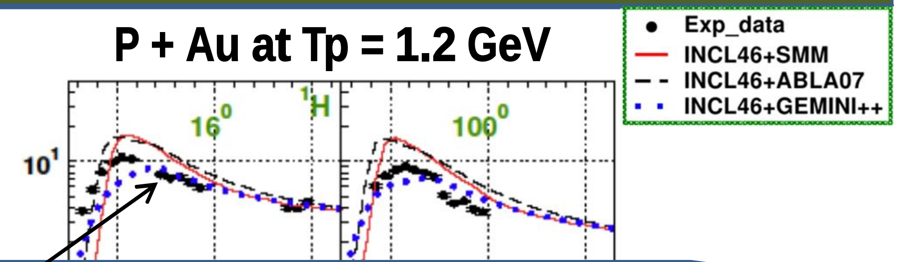
P+Au at Tp = 1.2 GeV for E <= 30 MeV

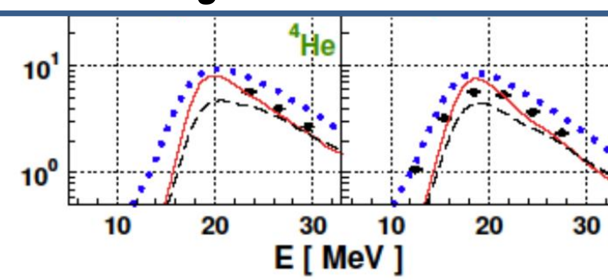


P+Au at Tp = 1.2 GeV for E > 30 MeV



P + Au at Tp = 1.2 GeV





What information we get:

- ***For protons GEMINI++ seems in better agreement than SMM and ABLA07.***
- ***Similarly, for other particles we can compare the deviations from the expected values by seeing the representative numbers***
- ***Deviations seem to be far from the range of agreement proposed by this test, still it can clearly help to predict which model is better among each other.***

- **We have presented a method to validate the theoretical model predictions to describe the experimental data (individually) in a quantitative way.**
- **The used deviation factor (ε) can provide ranking to theoretical models by judging their deviation from the expected values predicted by the different tests.**
- **The described method can be used to select the one among the others theoretical models, which is in better agreement with measurements.**
- **Here , we presented results only for selected targets and ejectiles. Work is in progress for other nuclear systems for the light charged particles and intermediate mass fragments measured by various collaborations.**

THANK YOU FOR YOUR ATTENTION