Results Production
and
Web site Tools

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OBJECTIVES of the "Benchmark of Spallation Models"

- **To assess the prediction capabilities of the spallation models** used or that could be used in the future in high-energy transport codes.
- **To understand the reason for the success or deficiency of the models** in the different mass and energy regions or for the different exit channels
- **To reach a consensus, if possible,** on some of the physics ingredients that should be used in the models.

Way to achieve the goals/meet the targets

- ✓ **Selection of an agreed set of experimental data for benchmarking of spallation models (Done in TRIESTE)**
- ✓ **Collections of calculations data corresponding to expt. ones (Done in IAEA and CEA-Saclay)**
- ✓ **Develop tools to perform the inter-comparison study (Done in IAEA and CEA-Saclay)**
- ✓ **Analyze the results to meet the objectives**

Status of Participants/Codes

Codes	Neutron	neutron multi.	Lcp	Pion	Residue	Excfn	Add. Info.	Ingre-dients
CEM03-02								
CEM03-03								
Cascade-04								
PHITS-jam								
PHITS-bertini								
PHITS-jqmd								
Isabel-smm								
Isabel-gemini++								
Geant4-bertini								
Geant4-binary								
Cascade-asf								
Incl4.5-abla07								
Incl4.5-smm								
isabel-abla07								
Incl4.5-gemini++								
Cascade-x								
MCNPX-bert								

Why Additional information?

- **To understand the reason for success or deficiency**
- **Useful to analyze the results**

P_Fe_1200_info		CEM03-02	CEM03-03	Isabel-gemini	Isabel-smm
Reaction σ , (mb)		739.8	739.8		
σ for Norm, (mb)		744.4	744.31	733.752	739.41
Characteristics remnant nucleus					
Before preeq	E*av (MeV)	169.1	169.1	68.64	68.20
	Zav	24.5	24.5	24.61	24.62
	Aav	51.6	51.6	52.80	52.81
	Lav	7.0	7.0		
	E*/A (MeV)	3.42		1.33	1.32
	P_R (MeV/c)	525.8			
Before de-excitation	E*av (MeV)	143.3	147.3		
	Zav	24.0	23.9		
	Aav	50.6	50.5		
	Lav	7.9	8.1		
	E*/A (MeV)	2.98			
	PR (MeV/c)	518.5			
Multiplicities					
	Neutron (Mn)	5.546	5.4976	1.98 (de-exct)	2.23 (de-exct)
	Proton (Mp)	4.543	4.4905	1.31 (de-exct)	1.028 (de-exct)
	Deuteron (Md)	1.264	1.2444	0.154 (de-exct)	0.105(de-exct)
	Tritium (Mt)	0.2627	0.2596	0.0333 (de-exct)	0.0311 (de-exct)
	Helium-3 (Mhe3)	0.2307	0.2266	0.0133 (de-exct)	0.0185 (de-exct)
	Alpha (Mhe4)	0.7548	0.7429	0.274	0.174

Steps of performed work at IAEA & CEA

- ❑ Conversion (if needed) of unique format of all data files
- ❑ Creation of scripts and/or develop programs for plotting of
- ▪ Double differential cross section
  - → Neutron production
  - → Light charged particle production
  - → Pion production
- ▪ Neutron multiplicity distribution
- ▪ Residue production
  - → Isotopic distribution
  - → Residue mass & charge production
- ▪ Excitation function
  - → Independent production of nuclides
  - → Cumulative production of nuclides

Used softwares for data processing

Plotting software : **gnuplot**
Language used : **Fortran, Perl**
System : **Unix**

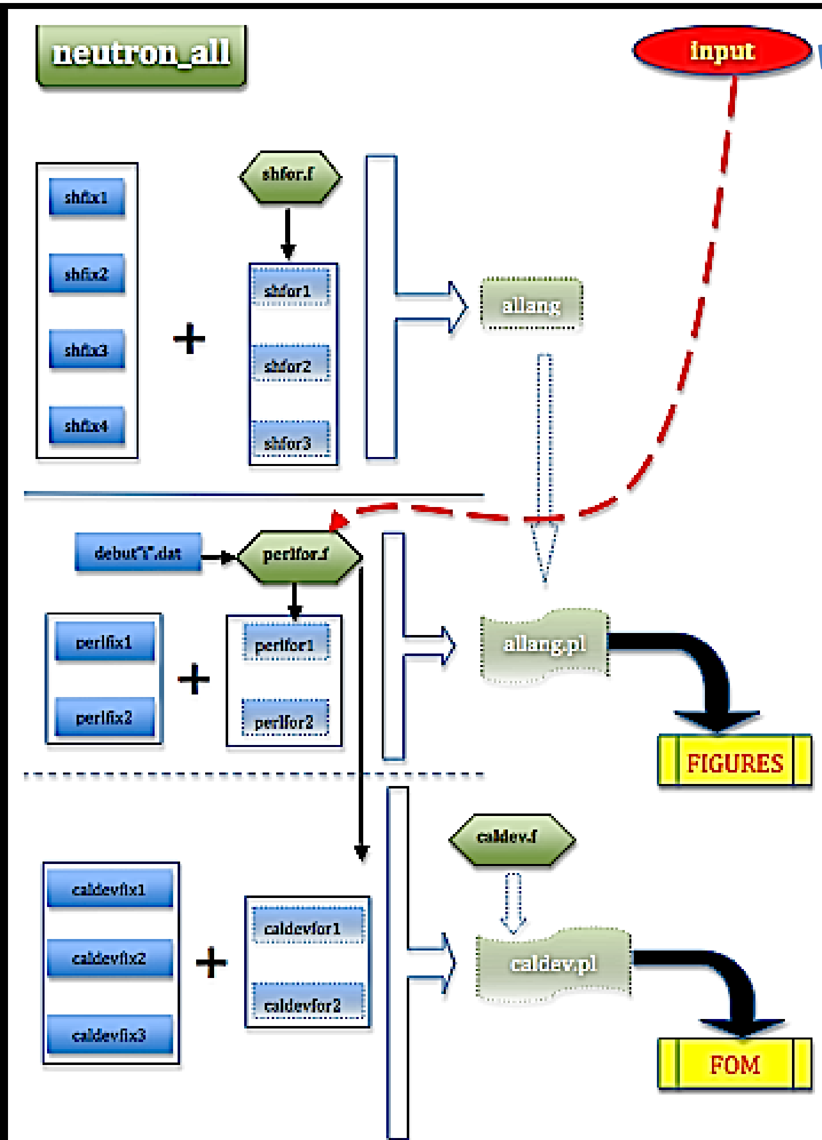
Creation of Scripts/ Developed programs

Several programs were written using FORTRAN and Perl languages to automatically generate the intercomparison figures, calculate deviation factors of experiment to calculated data, and generate figures with the deviation factors as

Experimental data
versus
Any combination of model calculations

Examples → Exp. data vs. all angle / model #1
→ Exp. data vs. all angle / model #1, #2, #3,..
→ Exp. data vs. one angle / model #1
→ Exp. data vs. one angle / model #1, #2, #3,..

Details description given in the preliminary report



exp. data	5
cem0302	1
cem0303	0
phits-bertini	0
phits-jam	0
cascade04	0
isabel-smm	0
g4bic	0
g4bert	0
isabel-gemini++	0
cascadeasf	0
incl45-abla07	0
incl45-smm	0
isabel-abla07	0
incl45-gemini++	0
phits-jqmd	0
cascadex	0
Mcnpx-bert-dres	0
model18	0
model19	0
model20	0
model21	0
model22	0
model23	0
model24	0
model25	0

Structure of the Presented Results in the Web Page

→Intercomparison Results [Fig.]
[data]

→Figs. by Figures of Merit [FoM]

Proj.	Targ.	En. proj. [MeV]	Exp. author	all models	cem03-02	phits-jam	geant4-bertini	cascade-asf	incl4.5-gemini	mcnpx-bert
n	Fe	65	hjort	[Fig.] [FoM]	[Fig.] [data] [FoM]	[Fig.] [data] [FoM]	[Fig.] [data] [FoM]	[Fig.] [data] [FoM]	[Fig.] [data] [FoM]	[Fig.] [data] [FoM]
p	Fe	800	leray	[Fig.] [FoM]	[Fig.] [data] [FoM]	[Fig.] [data] [FoM]	[Fig.] [data] [FoM]	[Fig.] [data] [FoM]	[Fig.] [data] [FoM]	[Fig.] [data] [FoM]

Contents (Available in the Spallations web page)

1. Neutron production

1.1 Double-differential Cross Section

Results have been produced for:

- **Each system of reaction**

  vs.

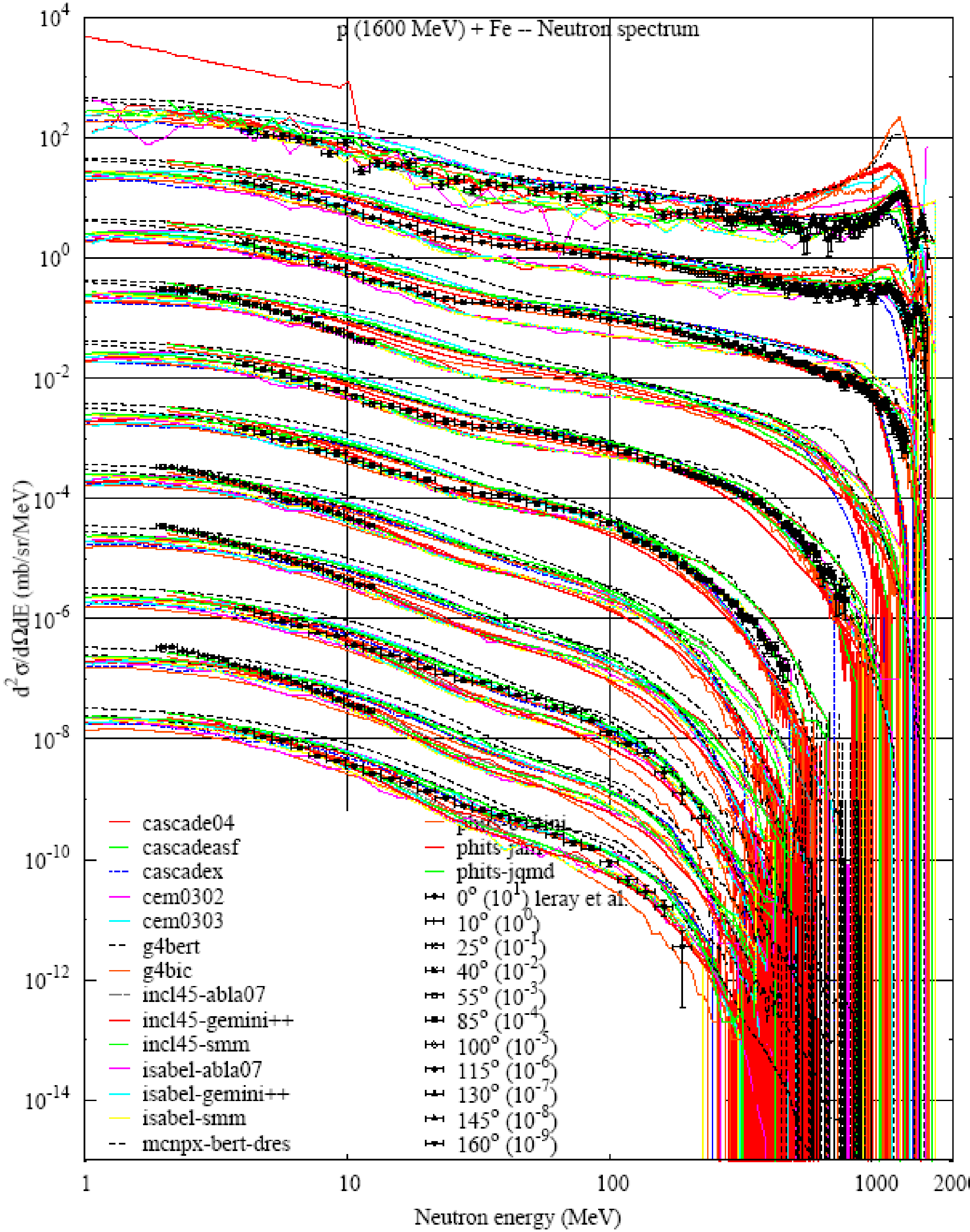
  All angle with one by one models (same scale)

- **Each system of reaction**

  vs.

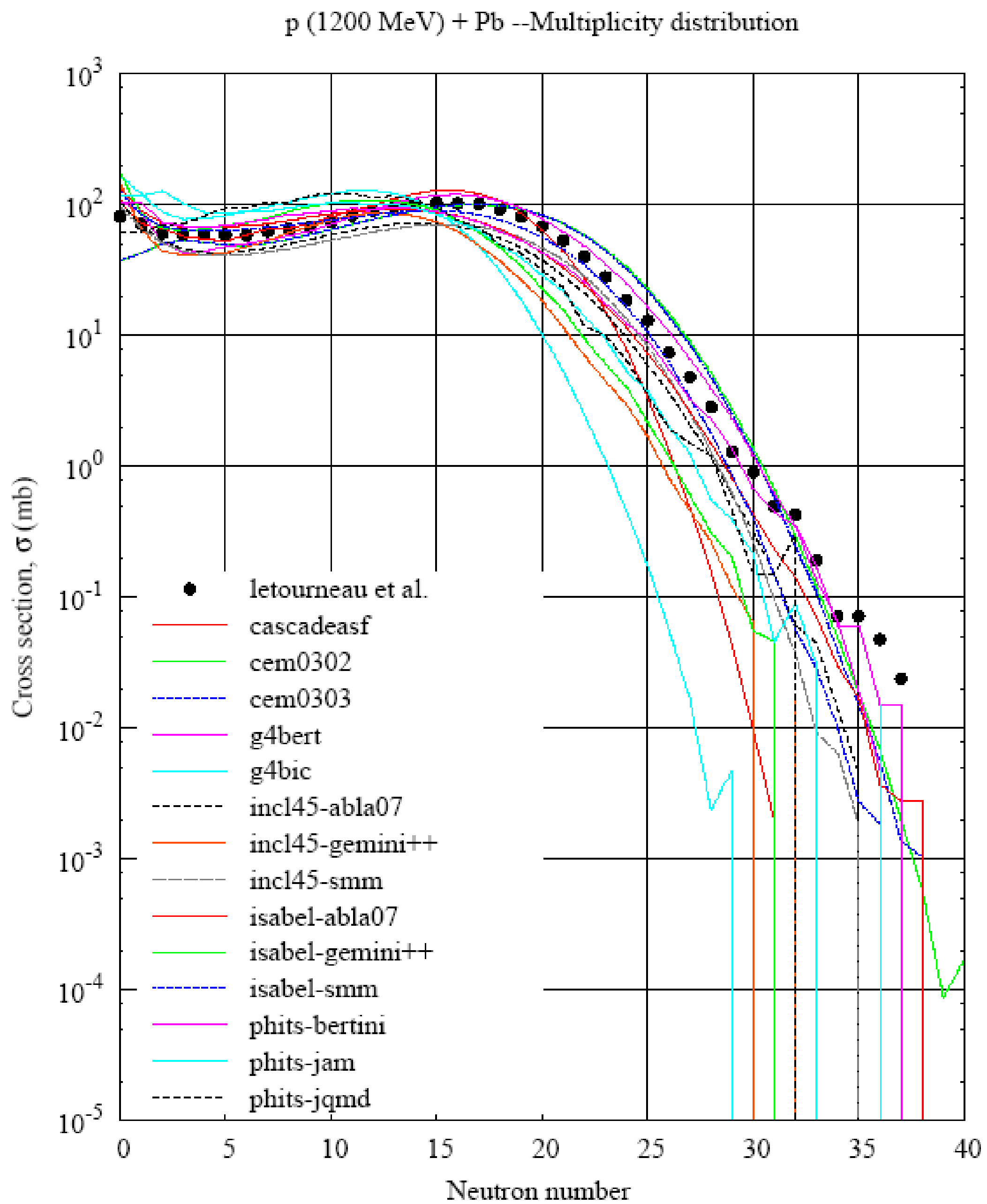
  All models with one by one angle

Neutron production



Multiplicity Distribution

Data were filtered by using Eff. function



1.3 Average Multiplicity (data generation)

Mean neutron multiplicity data has been generated from the neutron ddxs data files for each models :

Energy (MeV)	Energy bin (MeV)	Angle integrated, σ (mb/MeV)
E1	ΔE1	σ1
E2	ΔE2	σ2
E3	ΔE3	σ3
.		
.		
En	ΔEn	σn

Average multiplicity = $$\frac{\sigma_{E\min - E\max}}{\mathrm{Re}\, actionCrossSection}$$

Let, Emin (or E1) = 2 MeV
Emax (or En) = 20 MeV

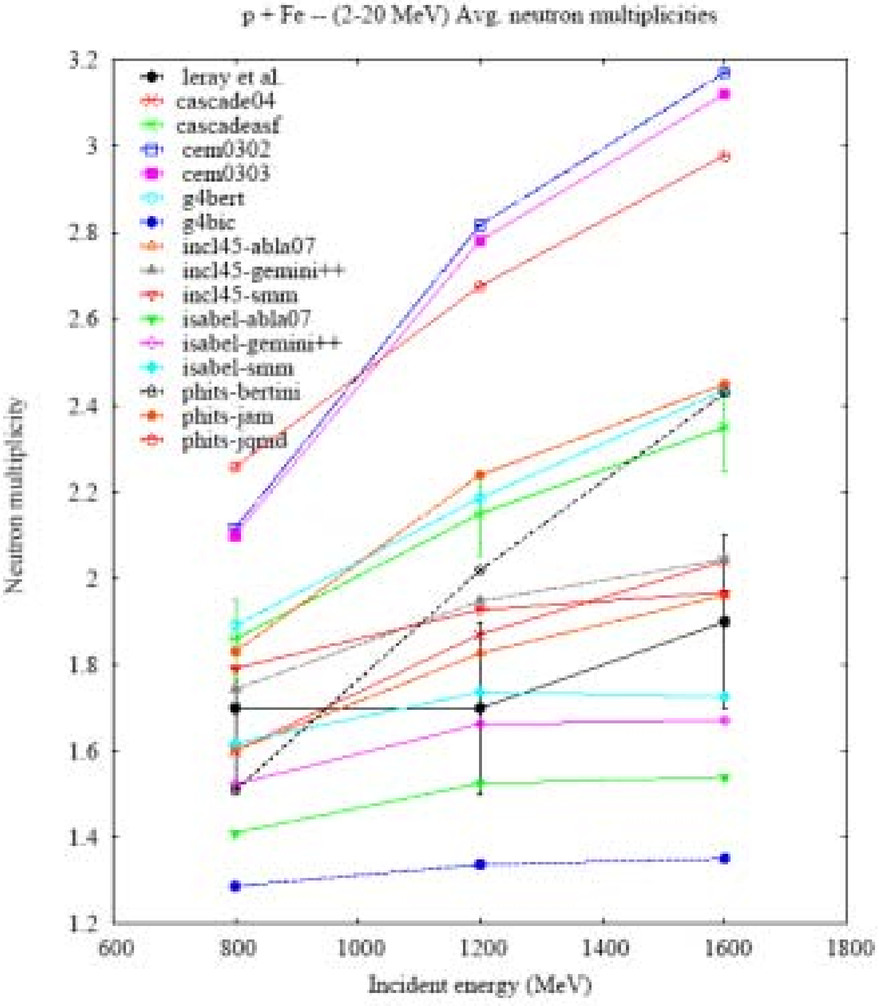
$\sigma_{2\text{-}20}$ MeV = (σ1* ΔE1 * 2) + (σ2* ΔE2* 2) + (σ3*ΔE3* 2)+ ....+ up to 20 MeV value [if ΔE is the half of the bin energy]

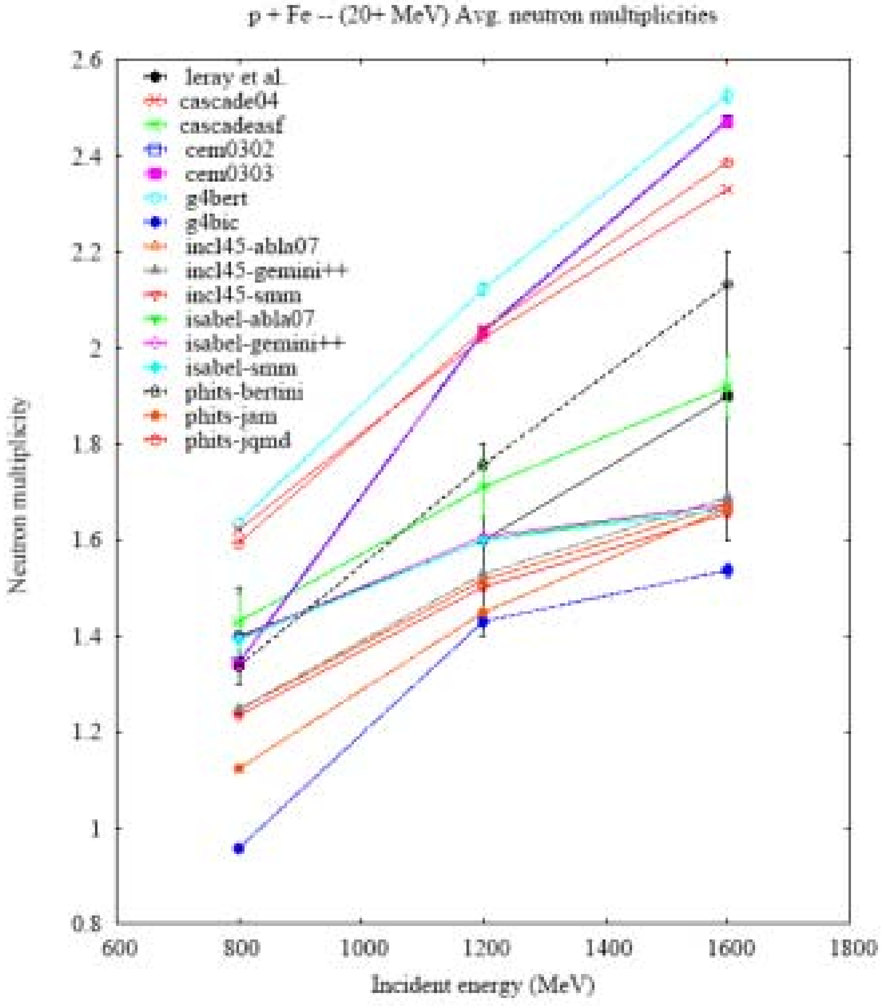
= (σ1* ΔE1) + (σ2* ΔE2) + (σ3*ΔE3)+ ....+ up to 20 MeV value [if ΔE is the full bin energy]

Average Multiplicity

→Neutron emission with 2-20 MeV

→Neutron emission with 20+ MeV





2. Light charged particle production

2.1 Double-differential Cross Sections

2.1.1 Proton

2.1.2 Deuteron

2.1.3 Tritium

2.1.4 Helium-3

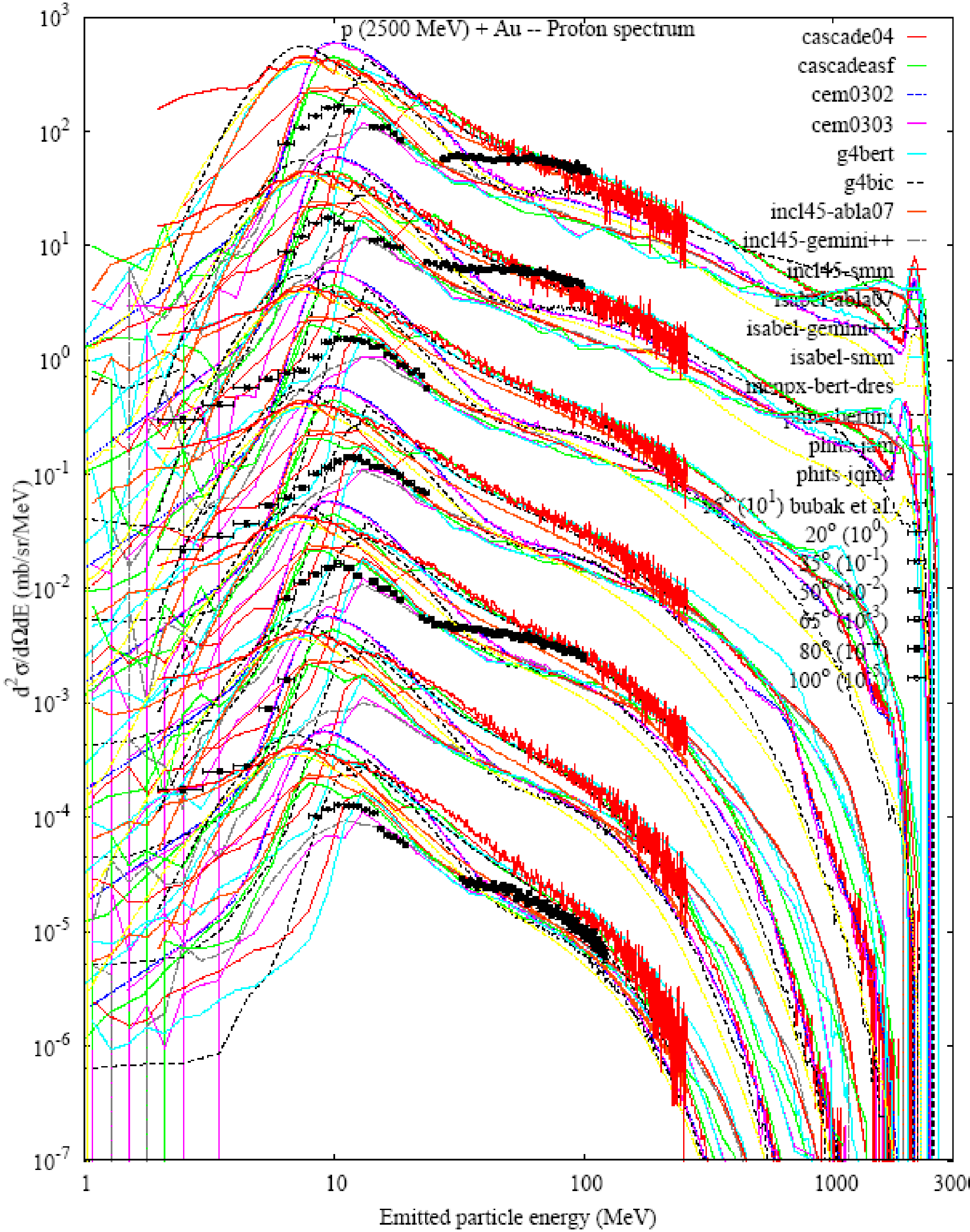
2.1.5 Helium-4

Results have been produced for:

- **each system of reaction**
  vs.
  all angle with one by one models (same scale)

- **each system of reaction**
  vs.
  all models with one by one angle

Example: Proton production



3. Pion production

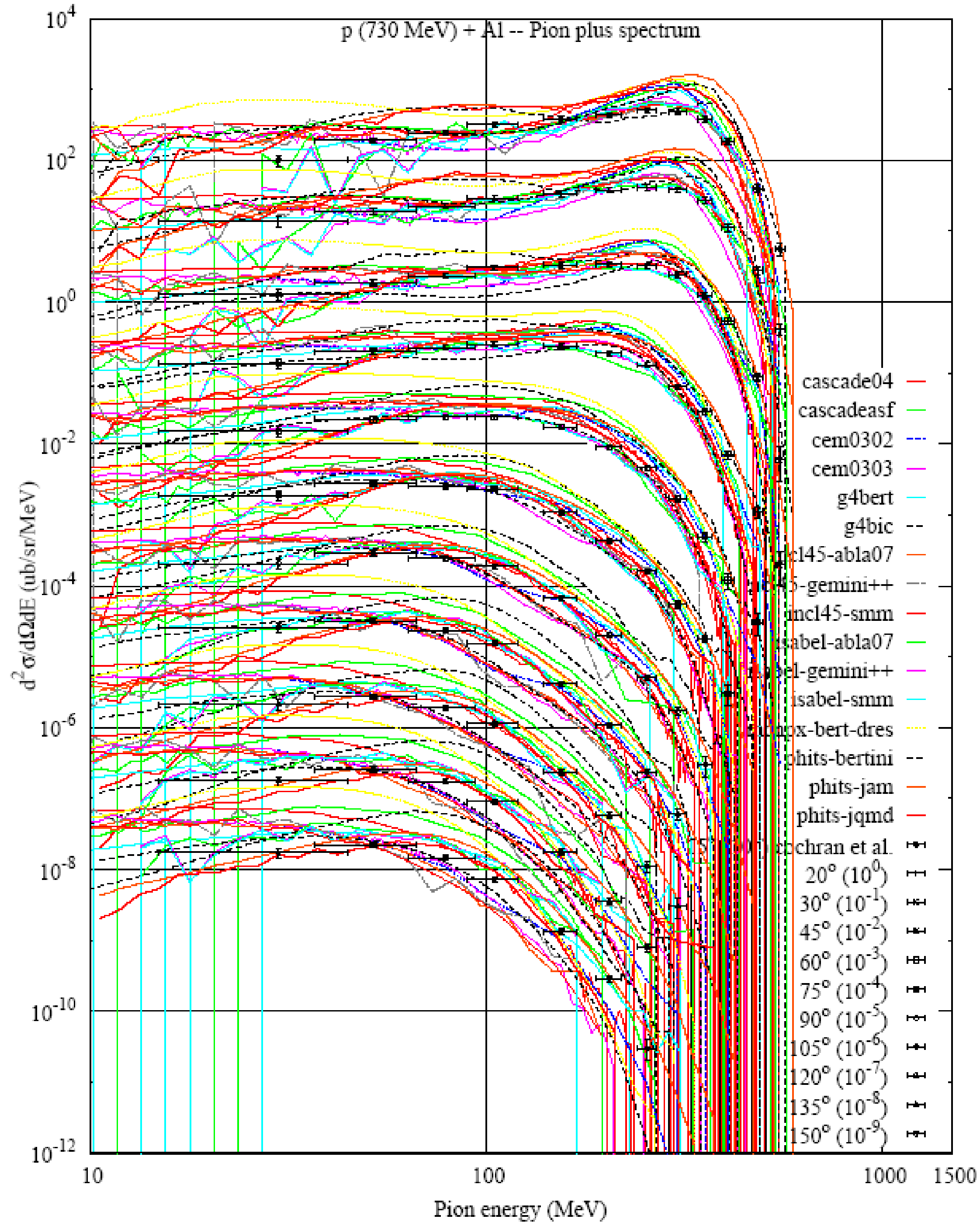
3.1 Pion plus
3.2 Pion minus

Results have been produced for:

- **each system of reaction**
  vs.
  all angle with one by one models (same scale)

- **each system of reaction**
  vs.
  all models with one by one angle

Pion production



4.1 Residue charge production (Generation of data)

▪Calculated nuclides which are exactly similar to the experimental nuclides were added for each particular **charge number.**

▪In the below table, the red marked nuclides were not reported in the experiment, and therefore, we neglected them to make an appropiate comparison.

Fe56_p_300_res_villagrasa (Expt.)				Model: CEM03-02			
Z	**A**	**Sig**	**+/-**	**Z**	**A**	**Sig**	**+/-**
27	54	0.092	0.0041	27	56	7.022	0.068
27	55	0.913	0.0341	27	55	3.764	0.049
27	56	1.390	0.0538	27	54	0.553	0.019
				27	53	0.021	0.004
				27	52	0.001	0.001

Added based on Z number			Added based on Z number		
Z	**Sig**	**+/-**	**Z**	**Sig**	**+/-**
27	0.239500E+01	0.965863E-01	27	0.113390E+02	0.248746E+00

Residue mass production (Generation of data)

▪Calculated nuclides which are exactly similar to the experimental nuclides were added for each particular **mass number.**

→ In the below table, the bold nuclides for specific mass number were added to make the total mass production data file.

Fe56_p_300_res_villagrasa (Expt.)				Model: CEM03-02			
Z	**A**	**Sig**	**+/-**	**Z**	**A**	**Sig**	**+/-**
27	**54**	**0.092**	**0.0041**	27	56	7.022	0.068
27	55	0.913	0.0341	27	55	3.764	0.049
27	56	1.390	0.0538	27	**54**	**0.553**	**0.019**
26	51	0.021	0.0010	27	53	0.021	0.004
26	52	0.554	0.0310	27	52	0.001	0.001
26	53	5.305	0.2462	26	56	16.124	0.102
26	**54**	**33.034**	**1.3291**	26	55	64.689	0.205
26	55	68.354	2.5454	26	**54**	**36.369**	**0.154**
25	49	0.020	0.0021	26	53	6.659	0.066
25	50	0.495	0.0372	26	52	1.053	0.026
25	51	5.855	0.3618	26	51	0.037	0.005
25	52	23.499	1.3254	26	50	0.001	0.001
25	53	52.470	2.4316	25	55	32.786	0.146
25	**54**	**55.001**	**4.6**	25	**54**	**36.056**	**0.153**
25	55	37.652	1.4019	25	53	41.567	0.164
25	56	0.088	0.0041	25	52	20.476	0.115
				25	51	6.038	0.063
				25	50	0.848	0.023
				25	49	0.017	0.003
				25	48	0.001	0.001
Added based on A number				**Added based on A number**			
A	**Sig**	**+/-**		**A**	**Sig**	**+/-**	
54	0.909750E+02	0.409331E+02		54	0.747120E+02	0.149465E+01	

4. Residue production (Reaction with inverse kinematics)

4.1 Residue charge production

(Particular Z – integrated cross sections)

4.2 Residue mass production

(Particular A – integrated cross sections)

Results have been produced for:

- **each system of reaction**

  vs.

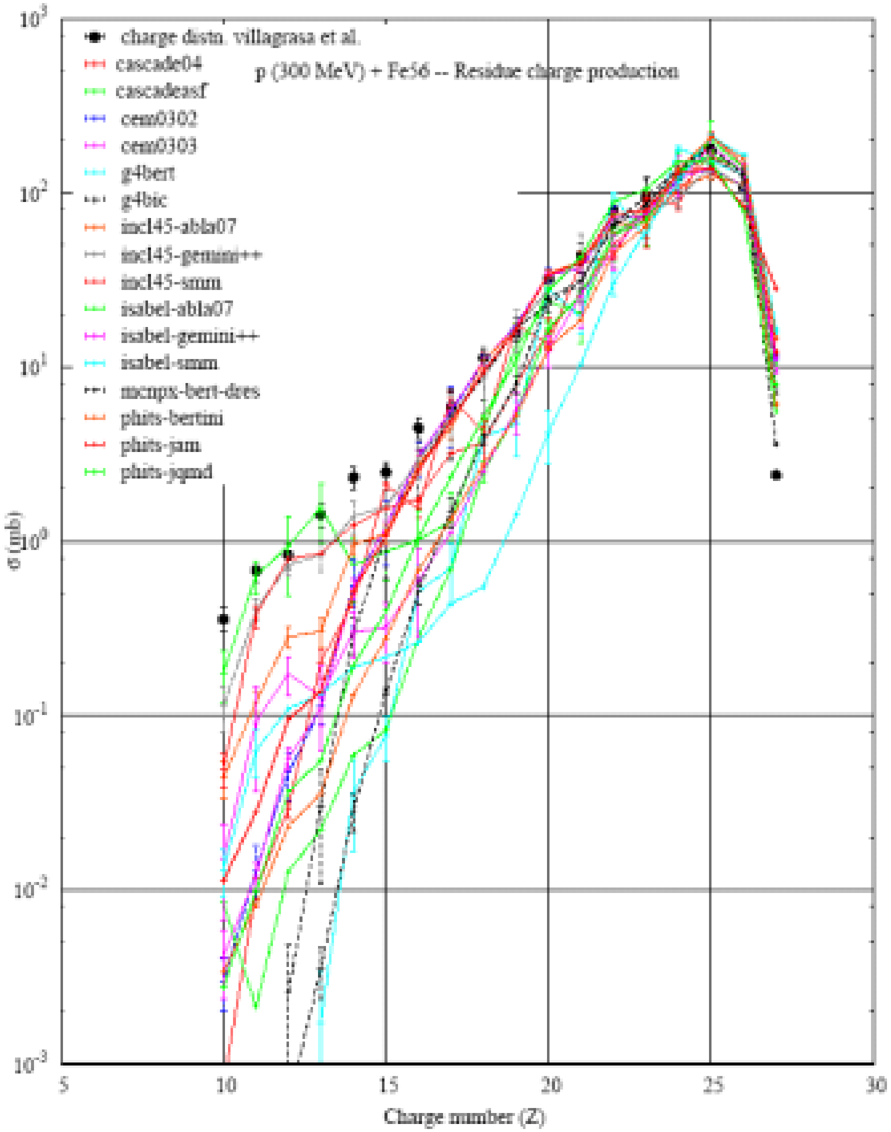
  charge/mass number with one by one models (same scale)

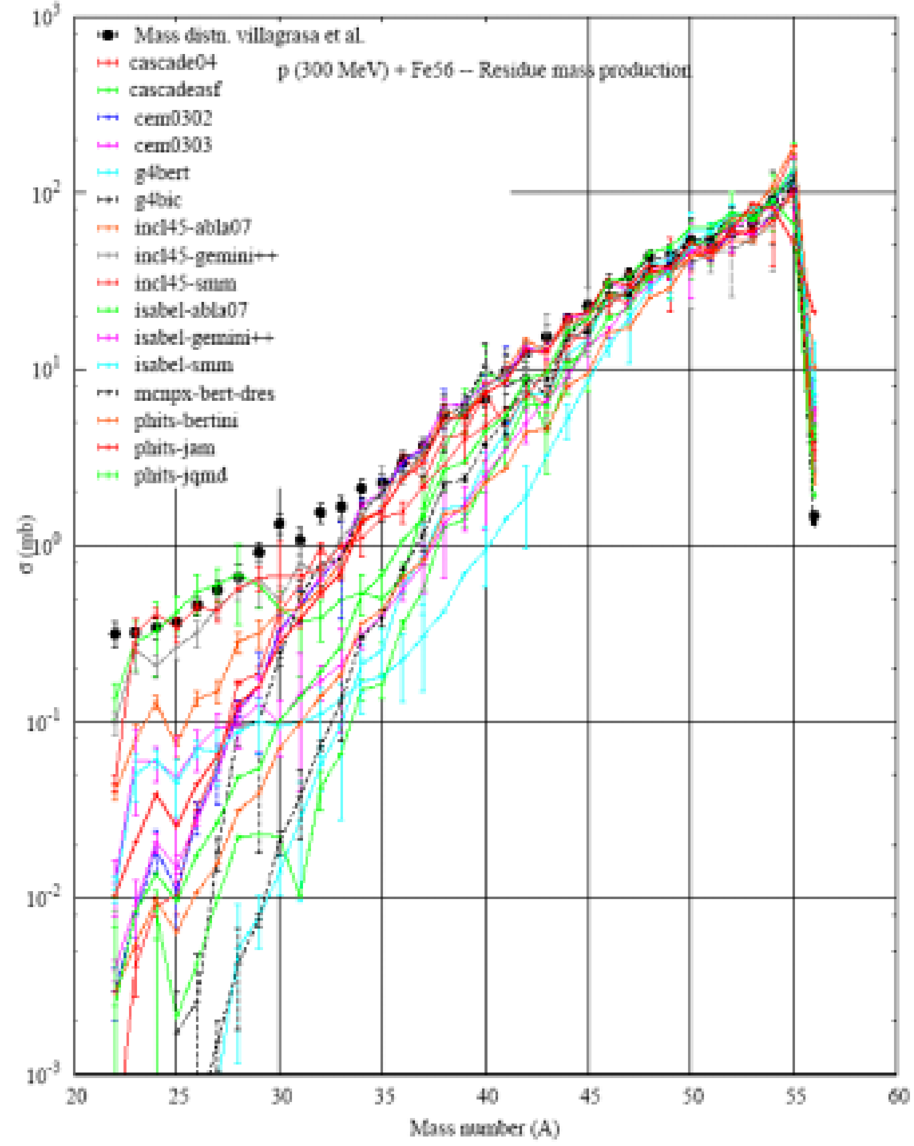
- **each system of reaction**

  vs.

  all models with charge/mass number

Residue production (Reaction with inverse kinematics)

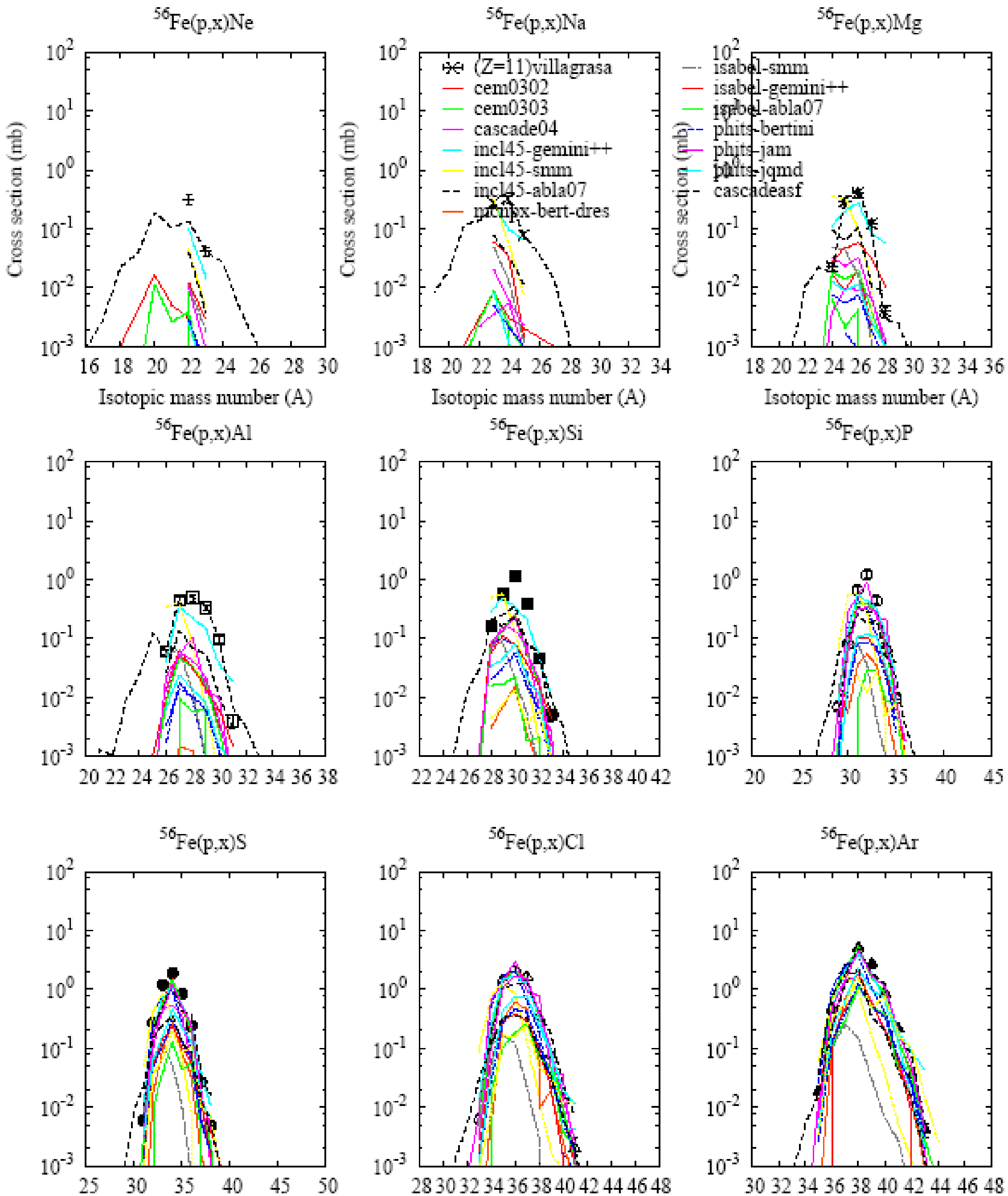




4. Isotopic distribution (Data generation)

- **Individual data files based on each charge number were extracted/generated both from the experimental and calculated data files.**
- **Individual figures were produced for each nuclides as expt. vs. each model**

Isotopic distribution (plotting)



5. Excitation function (Data generation & plotting)

- Excitation functions data were received in free format
- The measured nuclide production cross section can be either independent & cumulative types nuclides
- If the nuclide is produced only by the high-energy reaction, it is considered as independent.
- If the nuclide has been produced via high-energy interaction and decay of precursors, then it is considered as cumulative

- We developed tools to generate cumulative data using *DCHAIN-SP* library
- A comprehensive description has been posted in the web page about the cummulative production of nuclides
- Both the independent and cumulative nuclides production as function of incident energy were plotted individually with expt. vs. one by one models

Excitation function (Data generation)

Assuming only one hypothesis, which is that the half-life of the Mother is short compared to that one of the Daughter, the cumulative cross section is given by:

$$\sigma_{D,cum} = \sigma_{D,ind} + \sigma_M \frac{\lambda_M}{\lambda_M + \lambda_D}$$

where

- $\sigma_{D,cum}$ is the cumulative cross-section of the Daughter,
- $\sigma_{D,ind}$ is the independent cross-section of the Daughter,
- σ_M is the cross-section of the Mother (which can take into account grand-mother, etc.), and
- $\lambda_{M(D)}$ is half-life of the Mother (Daughter).

✓To perform cumulative calculations a code has been built which uses the above equation and doing the possible iterations (mother, grand mothers, etc.). This code needs a library, which contains the chains of precursors for all nuclides with necessary information that are branching ratio and half-life.

✓According to the meaning of "the half-life of the Mother is short compared to that one of the Daughter", some chains of precursors can change.

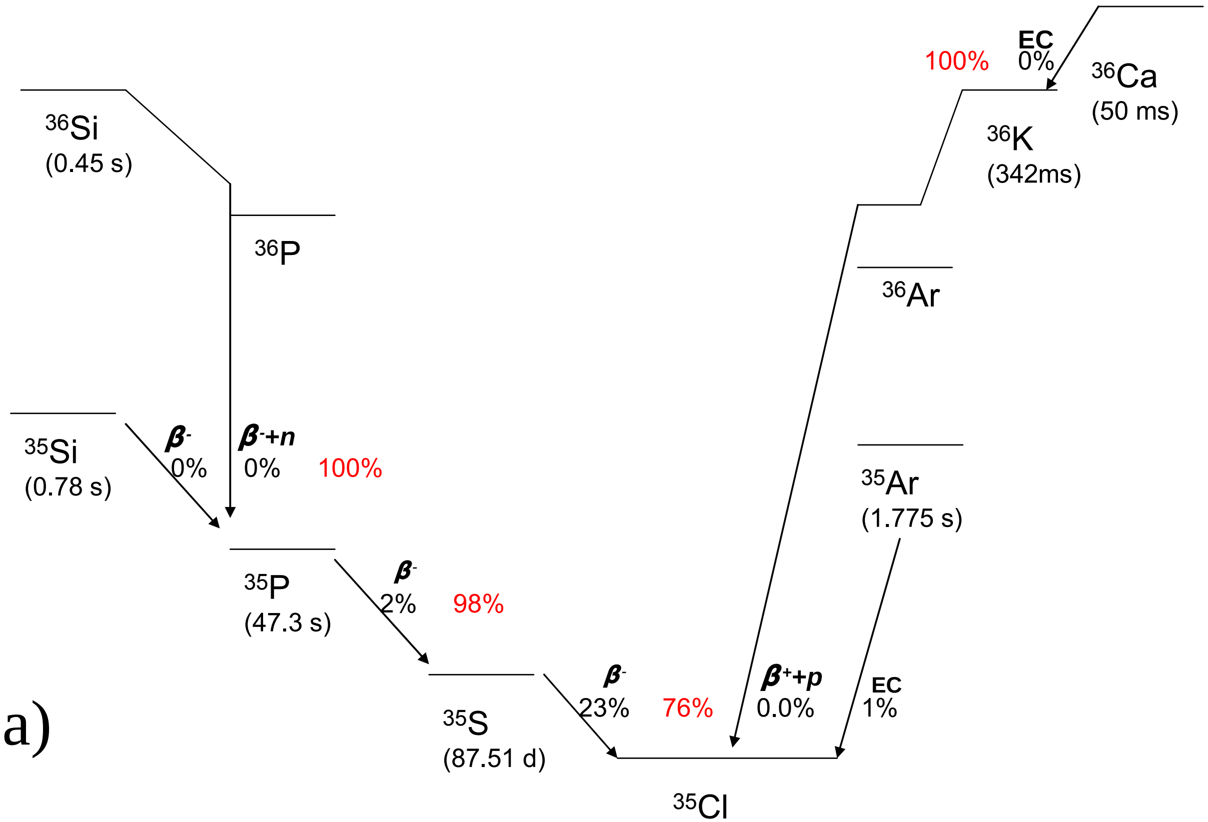
✓Information to create the library comes from the DCHAIN-SP library (JAERI-Data/Code 99-008)

Example, the chain obtained for 35Cl with lM / lD = 10.

35Cl has 3 mothers (35S, 35Ar and 36K).

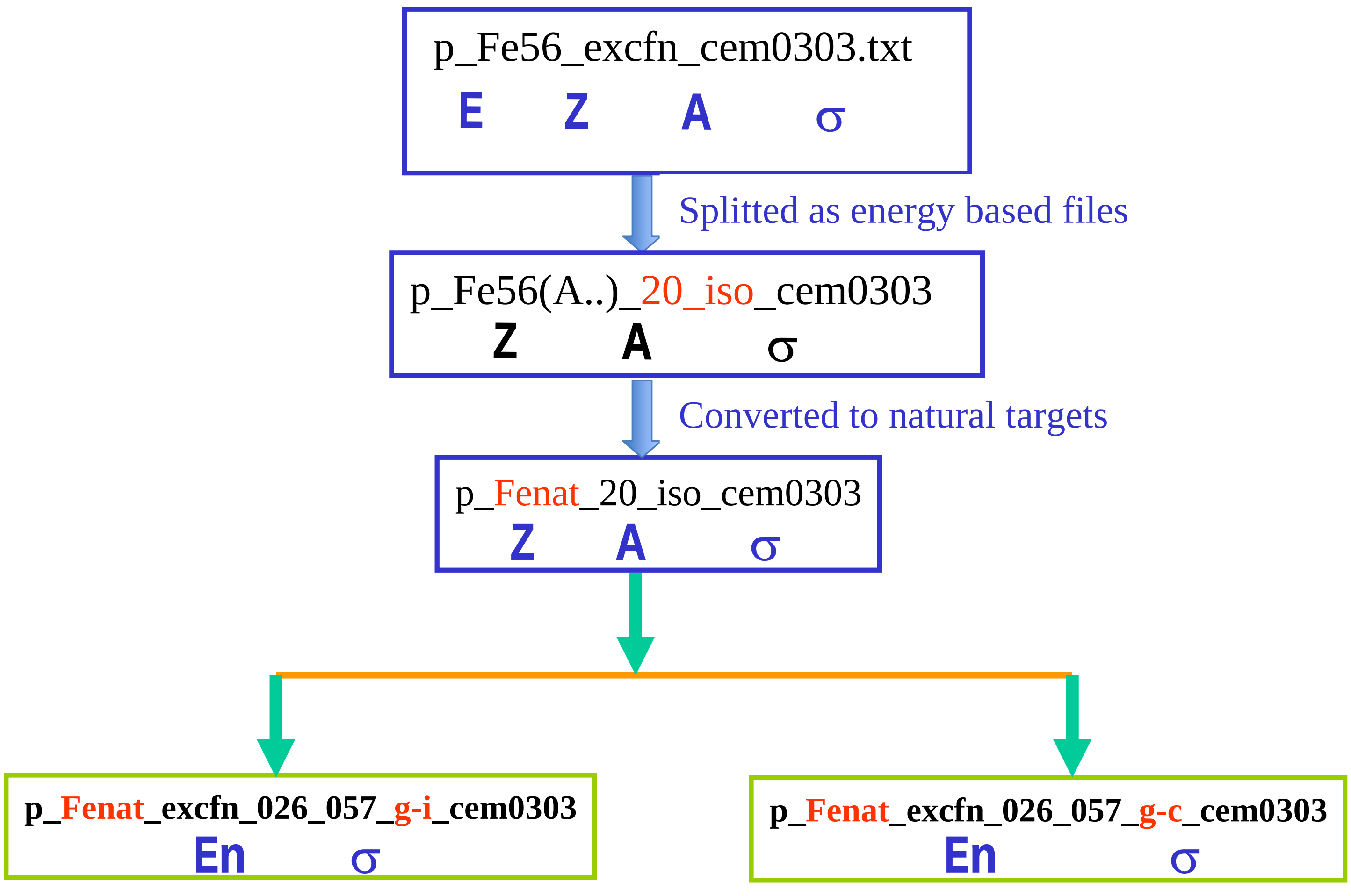
35S has 1 mother (35P), which has 2 mothers (35Si and 36Si).

Finally
35Ar has 1 mother (36Ca)

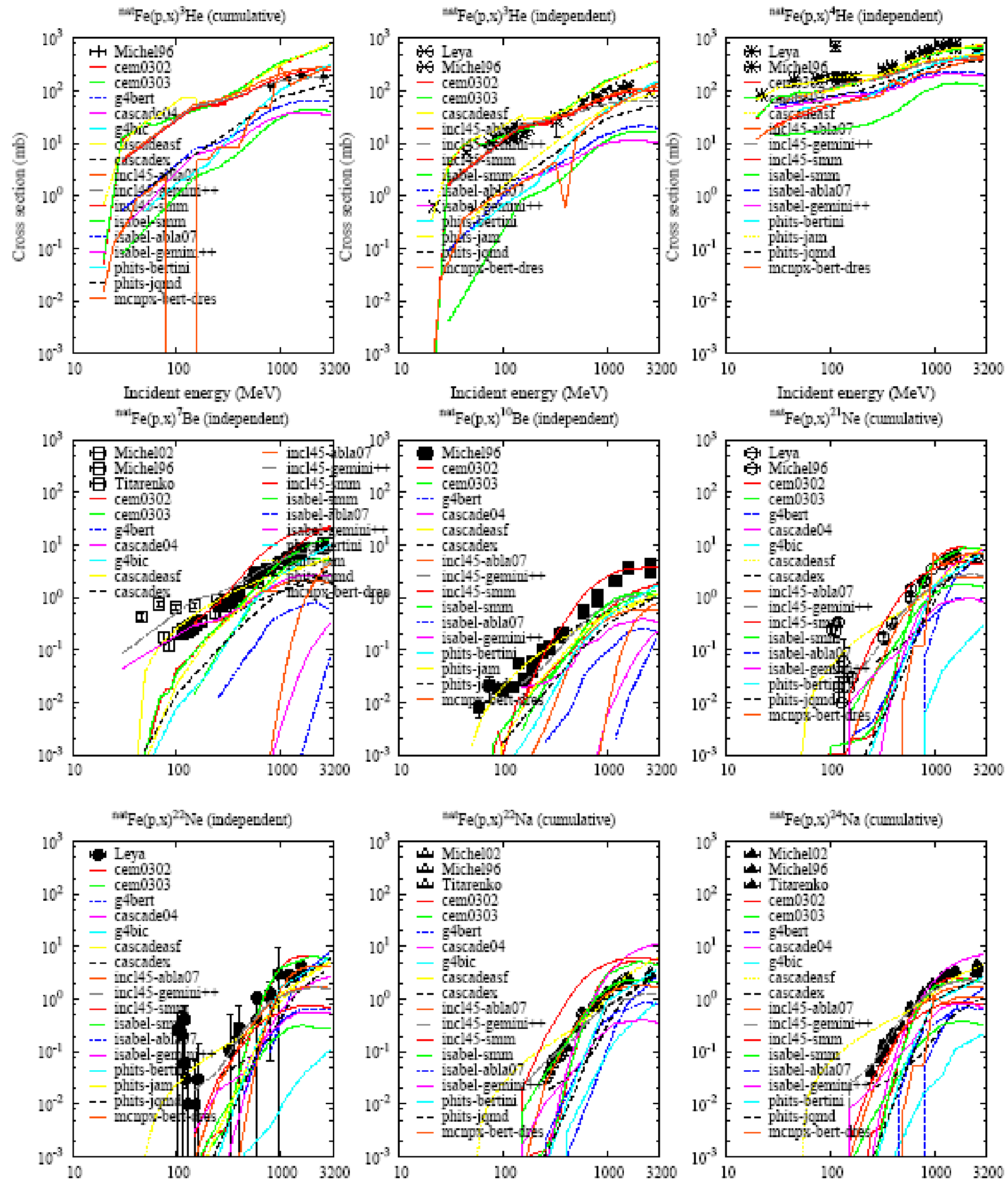


From this example,
76.3% of the 35Cl come from direct production and 23.7% from decays (22.51 from 35S, 1.19 from 35Ar and nothing from 36K).
Moreover, 35S is produced directly by reaction (98.13%), but also by decay of 35P (1.87%).

Excitation function (Data generation)



Excitation function
(Plotting)



Figures of Merit

Quantification of difference between results of calculations and measured data

Deviation factors

1. **Mean weighted deviation (similar to chi-square)**

or

H factor

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

[N. Kurenkov et al., 1999]

2. Ratio of calculated to experimental values

or

R factor

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

[C. Broeders et al., 2006]

3. Mean square deviation factor,

F factor

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

[R. Michel et al., 1997]

4. S factor [provided by A. Konobeyeev]

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

4. M factor [provided by R. michel]

The intrinsic discrepancy between the experimental and calculated cross sections is calculated by:

$$M = \min\left\{\sum_{i=1}^{n_{\exp}} \sigma_{\exp}(A_i)\log\frac{\sigma_{\exp}(A_i)}{\sigma_{\text{calc}}(A_i)}, \sum_{i=1}^{n_{\exp}} \sigma_{\text{calc}}(A_i)\log\frac{\sigma_{\text{calc}}(A_i)}{\sigma_{\exp}(A_i)}\right\}$$

For charge distributions replace *A* by *Z*

6. Additional values, P factors

$P_{1.3} = N_{1.3}/N, \quad N_{1.3} : \; 0.77 < \sigma_i^{calc} / \sigma_i^{exp} < 1.33$

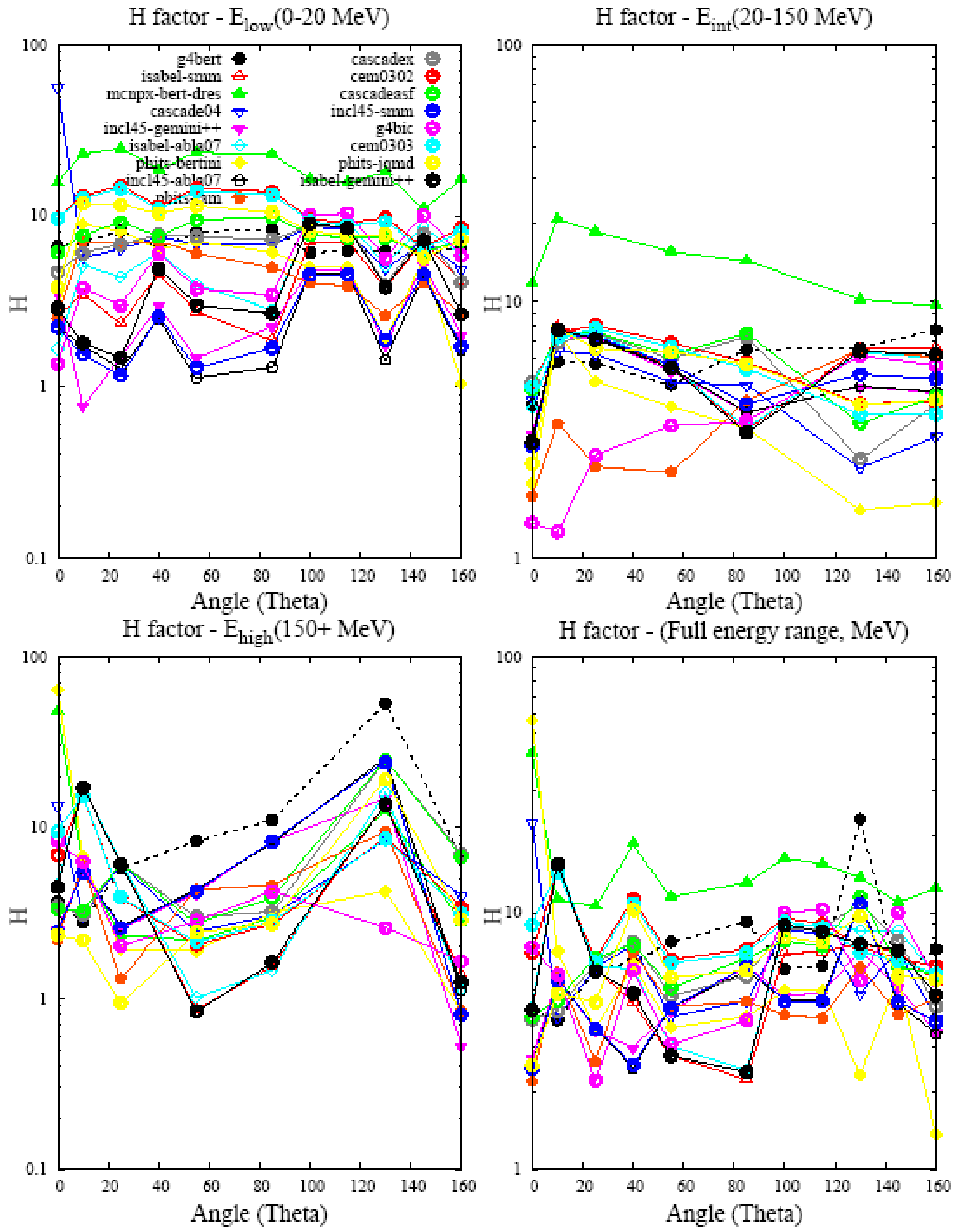
$P_{2.0} = N_{2.0}/N, \quad N_{2.0} : \; 0.50 < \sigma_i^{calc} / \sigma_i^{exp} < 2.0$

$P_{10.0} = N_{10.0}/N, \quad N_{10.0} : \; 0.1 < \sigma_i^{calc} / \sigma_i^{exp} < 10.0$

[Yu. E. Titarenko, ISTC 839B-99, 2001;
A. Yu. Konobeyev et al., Kerntechnik **73** (2008) 1-2]

Example: H factor

for the double differential cross section of natFe(p, xn) at 1.6 GeV



Preliminary outcomes for particle production

Neutron productions: Most of the models well reproduce the experimental data in both values and shape of the spectrum.

Neutron multiplicity distributions: Shows a general good reproduction for heavy target (e.g. Pb) but considerable discrepancy in light target (Fe).

Proton productions: Overall good reproduction of experimental data by some models, except few reaction systems.

Composite particles (d, t, He-3, He-4..) **productions:** Most of the models have deviation to experimental data around a factor of 2 or higher. This is even worse in case of low energetic reaction systems.

Pion productions: Shows an overall good reproduction of the experimental data by all models.

Preliminary outcomes for Residue

Residue mass and charge productions: Overall good reproduction of experimental data by most of the participated models, especially for heavy tagets (e.g., Pb, U).

Isotopic distributions: Overall good reproduction of experimental data by most of the participated models.

Exciatation functions of residual production cross sections: Only few models could reproduce well the experimental data.

Major outcomes on Performed work at IAEA and CEA-Saclay

- Necessary tools were developed to automatically generate the intercomparison figures for each experimental reaction systems with any combinations of model calculations.
- Tools were also developed for calculations of residue charge production, residue mass production, and isotopic distribution data , and and generation of cumulative productions of residual nuclei data.
- More than 10000 figures has been produced for both the qualitative and quantitative analyses of experiments to model calculations
- A well organised web page for this intercomparison exercise has been developed, and all generated figures and participated codes data has been posted

- We expect that the intercomparison results available in the web page critically helps the code developers to understand the successes and deficiencies of their codes.

Major outcomes on Performed work at IAEA and CEA-Saclay

A comprehensive explanation is available in the preliminary report on

Benchmark of Nuclear Spallation Models

Preliminary report

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Thank You !