



Benchmark of Spallation Models

Results of a global analysis: Residues

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- Mass and charge distributions
- Isotopic distributions
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International Code Comparison for Intermediate Energy Nuclear

Data, M. Blann, H. Gruppelaar, P. Nagel, J. Rodens, NEA/OECD, NSC/DOC(94)-2, Paris 1993

International Codes and Model Intercomparison for Intermediate Energy Activation Yields, R. Michel, P. Nagel, NEA/OECD, NSC/DOC(97)-1, Paris 1997

Participation in Intercomparison by Code Name and Physics Employed

Code Name	Physics
HECC/MECC7 + EVAP-F	INC+EVAP
GEANT	INC+EVAP
HERMES (HETC - KFA2)	INC+PE+EVAP
LAHET	INC+PE+EVAP
LAHET	INC+PE+EVAP
HETC-3 STEP	INC+PE+EVAP
CEM92M	INC+PE+EVAP
CEM92	INC+PE+EVAP
NUCLEUS	INC+EVAP+FERMI
	STATISTICS
ALICE92	PE+EVAP
ALICE87 MOD	PE+EVAP
ALICE F	PE+EVAP
PEQAQ2	PE (EVAP VIA
	MASTER EQ)
GNASH	EXCITON+HAUSER-
	FESHBACH EVAP
FKK-GNASH	FKK+EXCITON
	+EVAP (H-F)
KAPSIES+GRAPE	FKK+EVAP
QMD	INC+2 Body Forces
	Between Collisions
SYSTEMATICS	SYSTEMATICS

1993

Participation in Intercomparison by Code Name and Physics Employed 1997

code used	physical model employed
PEQAG2 (extended)	PE + EVAP via MASTER EQ.
ALICE 92	PE + EVAP
HMS-ALICE	HMS + EVAP
FKK-GNASH	FKK+EXCITON+HAUSER FESHBACH EVAP
QMDRELP+SDMRELP	QMD + SDM
HET/BRUYERE	INC + EVAP
PACE + MSM	INC + MSM
ISABEL-EVA	INC + EVAP
AREL	PE + EVAP (GDH)
HETC-FRG	INC + PE + EVAP + FRAGMENTATION
INUCL	INC + EVAP
MINGUS	FKK + EVAP
ISABEL/SMM	INC + SMM + EVAP
СЕМ 95	INC + PE + EVAP
HET-KFA2	INC + EVAP
SPALL (modified)/YIELD	TSAO & SILBERBERG SYSTEMATICS
ALICE - IPPE	PE + EVAP
CASCADE	INC + EVAP
DISCA	INC + EVAP
MSDM	INC + PE + SMM + EVAP + FERMI BREAKUP
HETC-3STEP	INC + PE + EVAP
MECC7 + EVAP_F	INC + EVAP

International Code Comparison for Intermediate Energy Nuclear Data M. Blann et al. (1993)

Double differential cross sections, (p,xn) and (p,xp) 20 MeV – 1600 MeV, Zr-90 and Pb-208

E incident	Angles
$25~{ m MeV}$	0° to 180° in 20° increments
$45~{ m MeV}$	0° to 180° in 20° increments
$80~{ m MeV}$	0°, 11°, 25°, 45°, 69°, 95°, 120°, 145°, 180°
$160~{ m MeV}$	0°, 11°, 25°, 45°, 69°, 95°, 120°, 145°, 180°
$256~{ m MeV}$	0°, 7.5°, 30°, 60°, 120°, 150°, 180°
$800~{ m MeV}$	0°, 7.5°, 30°, 60°, 120°, 150°, 180°
$1600~{ m MeV}$	0°, 7.5°, 30°, 60°, 120°, 150°, 180°



What is a factor of two among friends?





Zr-90(p,xn) @ 25 MeV





Pb-208(p,xn) @ 25 MeV



Pb-208(p,xn) @ 800 MeV



Conclusion

This exercise has, as a main goal, the display of results of model calculations versus high quality experimental data. Conclusions of such comparisons are subjective in nature. We have tried to attach a quite crude figure of merit for each entry at each energy and angle

From this exercise we may conclude that there is room for improvement in all codes, and that modelling calculations on a predictive basis may have uncertainties of the order of +50%.

. . .

The codes tested herein do well in reproducing many aspects of the microscopic nuclear physics, i.e., the DDCS. There is room for improvement and such efforts would be well spent given the importance of IEND for future technological development.

International Codes and Model Intercomparison for Intermediate Energy Activation Yields 1997

Blind intercomparison: E < 5 GeV Target elements: O, AI, Fe, Co, Zr, Au

code used	physical model employed
PEQAG2 (extended)	PE + EVAP via MASTER EQ.
ALICE 92	PE + EVAP
HMS-ALICE	HMS + EVAP
FKK-GNASH	FKK+EXCITON+HAUSER FESHBACH EVAP
QMDRELP+SDMRELP	QMD + SDM
HET/BRUYERE	INC + EVAP
PACE + MSM	INC + MSM
ISABEL-EVA	INC + EVAP
AREL	PE + EVAP (GDH)
HETC-FRG	INC + PE + EVAP + FRAGMENTATION
INUCL	INC + EVAP
MINGUS	FKK + EVAP
ISABEL/SMM	INC + SMM + EVAP
СЕМ 95	INC + PE + EVAP
HET-KFA2	INC + EVAP
SPALL (modified)/YIELD	TSAO & SILBERBERG SYSTEMATICS
ALICE -IPPE	PE + EVAP
CASCADE	INC + EVAP
DISCA	INC + EVAP
MSDM	INC + PE + SMM + EVAP + FERMI BREAKUP
HETC-3STEP	INC + PE + EVAP
MECC7 + EVAP_F	INC + EVAP

R. Michel, P. Nagel, NSC/DOC(97)-1, NEA/OECD, Paris, 1997



R. Michel, P. Nagel, NSC/DOC(97)-1, NEA/OECD, Paris, 1997

Deviation Factors as means of descriptive statistics

Define a mean square logarithmic deviation:

$$<(\log(\sigma_{\exp}) - \log(\sigma_{\text{theo}})^{2} >$$
$$= \sum_{i} (\log(\sigma_{\exp,i}) - \log(\sigma_{\text{theo},i})^{2} / NS$$

Average deviation factor for each reaction:

$$< F >$$

= $10^{\sqrt{\langle (\log(\sigma_{\exp}) - \log(\sigma_{theo})^2 \rangle}}$

Global mean deviation factor :

 $=10^{\sqrt{<<(\log(\sigma_{exp}) - \log(\sigma_{theo})^2)}}$

R. Michel, P. Nagel, NSC/DOC(97)-1, NEA/OECD, Paris, 1997

R. Michel, P. Nagel, International Codes and Model Intercomparison for Intermediate Energy Activation Yields, NSC/DOC(97)-1, NEA/OECD, Paris, 1997

Conclusion



On the average,

- predictions are at best within a factor of two;
- discrepancies reach more than a factor of ten.

Different predictions for individual reactions easily cover two orders of magnitude.

Goals of the present intercomparison

- to assess the prediction capabilities of the spallation models used or that could be used in the future in high-energy transport codes,
- to provide direct visual comparisons between data and calculation,
- to use quantitative measures such as Figures-of-Merit and deviation factors for the agreement between calculations and experimental data,
- 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.
- It is not the goal of the intercomparison to define "the best" model but for each observable, for different energy or mass range and to give recommendations to use one model rather than another one

Residual-nuclide-distribution cross sections measured in inverse kinematics by bombardment of hydrogen with heavy ions.

energy		reference
beam	in A MeV	
Fe	300	C. Villagrasa-Canton et al., Phys. Rev. C 75 (2007) 044603
Fe	1000	C. Villagrasa-Canton et al., Phys. Rev. C 75 (2007) 044603 P. Napolitani et al., Phys. Rev. C 70 (2004) 054607
Pb	500	L. Audouin et al., Nucl. Phys. A768 (2006) 1
Pb	1000	T. Enqvist et al., Nucl. Phys. A686 (2001) 481
U	1000	J. Taieb et al., Nucl. Phys. A 724 (2003) 413 M. Bernas et al., Nucl. Phys. A 725 (2003) 213 M. Bernas et al., Nucl. Phys. A765 (2006) 197 M. V. Ricciardi et al., Phys. Rev. C 73 (2006) 014607

Excitation functions of residual-nuclideproduction measured in classical kinematics

Tar- get	Energies in MeV	reference
Fe	20 – 2600	 R. Michel et al., Nucl. Instr. and Meth. B 103 (1995) 183 Th. Schiekel, R. Michel et al., Nucl. Instr. and Meth. B 114 (1996) 91 R. Michel et al., Nucl. Instr. and Meth. B 129 (1997) 153 R. Michel et al., Nucl. Sci. Tech., Supplement 2 (2002) 242 K. Ammon, I. Leya et al., Nucl. Instr. and Meth. B 266 (2008) 2 Yu.E. Titarenko et al., PRC 78 (2008) 034615
Pb	20 - 2600	M. Gloris et al., Nucl. Instr. and Meth. A463 (2001) 593 I. Leya et al., Nucl. Instr. and Meth. B229 (2005) 1 Y. E. Titarenko et al., Nucl. Instr. and Meth. A562 (2006) 801

Some heretical considerations:

Given the wealth of experimental information on residual nuclide production, we should be able to judge whether a model or code exhibits fundamental deficits in describing residual nuclide production.

Are such fundamental deficits potentially knock-out criteria for models and codes?

Such criteria could be the complete failure to describe

- Mass distributions,
- Charge distributions,
- Isotopic distributions,
- Energy dependencies.

Method of a Systematic evaluation



Categorization:

low energies		high energies		
Fe 300 MeV	Pb 500 MeV	Fe 1 GeV	Pb 1 GeV	U 1 GeV
target near products				
spallation products				
light products	light products	light products	light products	light products
-	-	-	fission products	fission products

Rating System for Mass, Charge and Isotopic Distributions

Categorization:

low energies		high energies		
Fe 300 MeV	Pb 500 MeV	Fe 1 GeV	Pb 1 GeV	U 1 GeV
target near products				
spallation products				
light products	light products	light products	light products	light products
-	-	-	fission products	fission products

There are no data for light complex nuclei. Light complex particles can only be taken into account by looking for the excitation functions.

Ratings:		
2	good	
1	moderately good , minor problems	
-1	moderately bad, particular problems	
-2	unacceptably bad, systematically wrong	

Mass Distribution of Residues



Mass Distribution of Residues



Mass Distribution of Residues at 1 GeV



Charge Distribution of Residues



Charge Distribution of Residues



Charge Distribution of Residues at 1 GeV



 10^{-2}

0

30

10⁻⁴

40 f0 Charge number (Z)

100

30

Mass and Charge Distribution of Residues from Uranium at 1 GeV



Mass distributions

Mass Distribution of Residues Iron @ 300 MeV



Mass Distribution of Residues Iron @ 1 GeV



Mass Distribution of Residues Lead @ 500 MeV



Mass Distribution of Residues Lead @ 1 GeV



Mass Distribution of Residues Uranium @ 1 GeV



Charge distributions
Charge distribution I ron @ 300 MeV



Charge distribution I ron @ 1 GeV



Charge distribution Lead @ 500 MeV



Charge distribution Lead @ 1 GeV



Charge distribution Uranium @ 1 GeV



Rating of the results of 15 participants for predicting the mass and charge distributions measured by inverse kinematics for iron, lead, and uranium at all energies



Possible maximum: 56 points

I sotope distributions

Exemplary isotope distributions for spallation products and target near products; iron 300 MeV and 1 GeV



Exemplary isotope distributions for spallation products and target near products; lead 500 MeV



Exemplary isotope distributions for light products, fission products, spallation products, and target near products; lead at 1 GeV



Exemplary isotope distributions for light products, fission products, spallation products, and target near products; uranium 1 GeV



Rating of the results of 15 participants for predicting the isotope distributions measured by inverse kinematics for iron, lead, and uranium at all energies.



Possible maximum: 28 points

Rating of the results of 15 participants for predicting the mass, charge, and isotope distributions measured by inverse kinematics for iron, lead, and uranium at all energies.



Possible maximum: 84 points

Excitation Functions

For excitation functions the simple rating system cannot be applied. The energy dependencies have to be looked at in detail.

The Benchmark on Spallation Models provides a tool for continuous improvement of models and codes and for iterative comparisons.

Excitation Functions Order of Presentation

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

Excitation Functions Iron















 10^{-2} 10^{-2} 10^{-6} 1000 3200 1000 3200

1000 3200





Excitation Functions Lead






















Xe-127 from lead

10

100

1000 3200















Bi-204 from lead



Statistical Factors

Mean deviation factor F exctation functions iron



Mean deviation factor F exctation functions iron



without mcnpx-bert

Mean deviation factor F exctation functions lead



F factor

Mean deviation factor F exctation functions lead



without mcnpx-bert

F-Factor



The Concept of Intrinsic Discrepancy

I propose to replace

the mean deviation factor

by the intrinsic discrepancy between

the experimental and theoretical PDFs.

PDF = probability density function

The Concept of Intrinsic Discrepancy

The intrinsic discrepancy $\delta\{p_1,p_2\}$ is a very general measure of the divergence between two distributions of the random vector **x** described by their density functions p_1 and p_2 :

$$\delta\{p_1, p_2\} = \min\left\{\int p_1(x) \ln \frac{p_1(x)}{p_2(x)} dx, \int p_2(x) \ln \frac{p_2(x)}{p_1(x)} dx\right\}$$

J.M. Bernardo, Bayesian Statistics, in: *Probability and Statistics* (R. Viertl, ed.) *Encyclopedia of Life Support Systems* (EOLSS). Oxford, UK: UNESCO, 2003.

Cross Sections: Excitation functions as PDFs

Let $\sigma(E)$ be integrable in a given energy interval $[E_{\min}, E_{\max}]$, then :

$$\sigma'(E) = \frac{\sigma(E)}{E_{\max}} = f(E)$$
$$\int_{E_{\min}} \sigma(E) dE$$

is a PDF for a reaction to occur as a function of energy *E*.

The Concept of Intrinsic Discrepancy applied to residual nuclide production

$$\sigma'_{\exp}(x) = \frac{\sigma_{\exp}(x)}{\underset{x_{\min}}{x_{\max}}} \quad \sigma'_{calc}(x) = \frac{\sigma_{calc}(x)}{\underset{x_{\min}}{x_{\max}}}$$

$$\delta\{\sigma'_{\exp}(x), \sigma'_{calc}(x)\} = \\ \min\left\{\int \sigma'_{\exp}(x) \ln \frac{\sigma'_{\exp}(x)}{\sigma'_{calc}(x)} dx, \int \sigma'_{calc}(x) \ln \frac{\sigma'_{calc}(x)}{\sigma'_{\exp}(x)} dx\right\}$$

with $x = E, A, Z, ...$

The Concept of Intrinsic Discrepancy applied to excitation functions

$$\sigma'_{\exp}(E) = \frac{\sigma_{\exp}(E)}{\int\limits_{E_{\min}}^{E_{\max}} \sigma_{\exp}(E) dx} \qquad \sigma'_{calc}(E) = \frac{\sigma_{calc}(E)}{\int\limits_{E_{\min}}^{E_{\max}} \sigma_{calc}(E) dx}$$

$$\delta\{\sigma'_{\exp}(E), \sigma'_{calc}(E)\} = \\\min\left\{\int \sigma'_{\exp}(E) \ln \frac{\sigma'_{\exp}(E)}{\sigma'_{calc}(E)} dx, \int \sigma'_{calc}(E) \ln \frac{\sigma'_{calc}(E)}{\sigma'_{\exp}(E)} dx\right\}$$

$$\delta\{\sigma_{\exp}'(E), \sigma_{calc}'(E)\} = \\ \min\left\{ \begin{cases} \int \sigma_{\exp}'(E) \ln \frac{\sigma_{\exp}(E)}{\sigma_{calc}(E)} dE + \ln \frac{\int \sigma_{calc}(E) dE}{\int \sigma_{\exp}(E) dE} \\ \int \sigma_{calc}'(E) \ln \frac{\sigma_{calc}(E)}{\sigma_{\exp}(E)} dE + \ln \frac{\int \sigma_{\exp}(E) dE}{\int \sigma_{calc}(E) dE} \\ \end{pmatrix} \right\}$$

Intrinsic Discrepancy: Characteristics

- It may be shown that the intrinsic divergence is symmetric, non-negative, and it is zero if, and only if, p₁(x) = p₂(x) almost everywhere.
- The intrinsic discrepancy is invariant under one-to-one transformations of x.
- > Besides, it is additive: if $x = \{x_1, \dots, x_n\}$ and

$$p_i(\mathbf{x}) = \prod_{j=1}^n q_i(x_j)$$
, then $\{p_1, p_2\} = n \{q_1, p_2\}$

Last, but not least, it is defined even if the support of one of the densities is strictly contained in the support of the other.

Intrinsic Discrepancy: Characteristics

The intrinsic discrepancy serves to define a useful type of convergence; a sequence of PDFs

${p_i(\mathbf{x})}_{i=1}^{\infty}$ converges intrinsically to a PDF $p(\mathbf{x})$ if (and only if)

 $\lim_{i\to\infty} \delta(p_i, p) = 0$

i.e., if (and only if) the sequence of the corresponding intrinsic discrepancies converges to zero.

Benchmark of Spallation Models Results of a global analysis: Residues

Conclusion

There is hope, but there is still room for improvements.

Deviation Factors

H-Factor



R-Factor

p (300 MeV) + Fe56 -- Residue charge production



D-Factor

p (300 MeV) + Fe56 -- Residue charge production



