MODELS AND CODES FOR SPALLATION NEUTRON SOURCES

Title:

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Models and Codes for Spallation Neutron Sources
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Models and Codes for intermediate Energy Nuclear Reactions
• Overview

• Evaporation

• Fission Models

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• Intranuclear Cascade

• Multifragmentation, Fermi Breakup

• Semiempirical Systematics

• High-Energy Transport Codes

• Further Work
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<td>RQMD</td>
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<td>RAL model</td>
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<td>ORNL model</td>
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</table>

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Multifragmentation
Evaporation models

Classical:


Quantum-Mechanical:


Reviews:


High Energy Fission


**Statistical Models of Fission:**


**Dynamical Models of Fission:**


**Semi-Phenomenological Models:**


Sequential binary decays using the code GEMINI:


Reviews:


**Pre-Equilibrium Models**

(*> 100 modifications*)

**Semi-Classical, Exciton and Hybrid models:**


**Reviews:**


**Quantum-Mechanical, MSC and MSD:**


**Review:**

Intranuclear Cascade Models (INC)


\[ N, \pi + A: \]


\[ A + A : \]


\[ \gamma + A : \]


\[ \bar{N} + A : \]


...
Reviews:


Multifragmentation

- Probabilistic models
  - Macroscopic statistical models
  - Microscopic dynamical models
  - Molecular Dynamics; Quantum Molecular Dynamics
  - Kinetic models
  - Sequential evaporation or very asymmetric fission
  - Hybrid models
  - ...

Reviews:


In MCNPX, we use only Fermi Breakup:


Ultrarelativistic energies

\textit{Gribov-Regge theory} (Perturbative QCD doesn’t apply yet)

- Quark Gluon String Model (QGSM)
- String Gas Model (SGM)
- Dual Parton Model (DPM)
- QCD Parton Model (PCM)
- Relativistic Quantum Molecular Dynamics (RQMD)
- HERWIG, ISAJET, PYTHIA, VECBOS, PAPAGENO, ..., event generators
- CALOR89 code
- Lund FRITIOF code
- VENUS (Very Energetic Nuclear Scattering) code
- GEANT4 code
- MARS code
- FLUKA (FLUctuating KAscade code)
- ...

\textbf{Reviews:}


Semiempirical Systematics

Reviews:


Recent Useful Systematics:


B. S. Sychev, *Cross Sections of High Energy Hadron Interactions on Nuclei* (Russian Academy of Science, Moscow Radiotechnical Institute, Moscow, 1999).
CASCADE

\[ f^{\text{cas}}(\vec{r}, \vec{p}, t) \equiv N_0 \delta(\vec{p} - \vec{p}_0) \exp \left[ - \int_0^t dt' \rho^{\text{T}} < \sigma_{\text{rel}} \right] + \]

\[ + \int_0^t dt'' \rho^{\text{cas}}(\vec{r} - \frac{\vec{p}}{m}(t - t''), t'') Q(\vec{r} - \frac{\vec{p}}{m}(t - t''), \vec{p}, t'') \exp \left[ - \int_{t''}^t dt' \rho^{\text{T}} < \sigma_{\text{rel}} \right] \]

\[ Q(\tau, p, t) = \int d\vec{p}_1 d\Omega_{\text{rel}} \frac{d\sigma_{\text{rel}}}{d\Omega}(v_{\text{rel}}) f^{\text{cas}}(\vec{r}, \vec{p}_1) f^{\text{cas}}(\vec{r}, \vec{p}_1, t); \quad j \equiv n, p, n^+, n^0, n^- \]

\[ \mathcal{P} = 0.3 \quad \downarrow \quad A, Z, E, n = p + h, \vec{P}, \vec{L} \]

PREEQUILIBRIUM

\[ \frac{\partial P(E, n, t)}{\partial t} = \lambda_+(n - 2, E) P(E, n - 2, t) + \lambda_0(n, E) P(E, n, t) + \]

\[ + \lambda_-(n + 2, E) P(E, n + 2, t) + \]

\[ + \sum_j \int dT \int dE' \lambda_j^2(n, E, T) P(E', n + j, t) \delta(E' - E - B_j - T) - \]

\[ - [\lambda_+(n, E) + \lambda_0(n, E) + \lambda_-(n, E) + \sum \Gamma_j(n, E)] P(E, n, t) \]

\[ \lambda_{\Delta n}(n, E) = \frac{2\pi\hbar}{\hbar} |M_{\Delta n}|^2 \omega_{\Delta n}(n, E); \quad \quad |M|^2 \sim \frac{< \sigma_{\text{rel}} > \sigma_{\text{rel}}}{V_{\text{int}}} \]

\[ \Gamma_j(n, E) \sim \int \frac{\omega(n - n_j, E - B_j - T)}{\omega(n, E)} T dT; \quad j \equiv n, p, d, t, 3 He, \alpha \]

\[ [n = \bar{n}] \quad \downarrow \quad A, Z, E, \vec{P}, \vec{L} \]

EQUILIBRIUM (COMPOUND)

\[ \omega(E) = \sum_n \omega(n, E) \sim \exp 2\sqrt{aE} \]

\[ a = a(Z, N, E) \sim A/10; \quad j \equiv n, p, d, t, 3 He, \alpha; \quad (+ \text{ fission}) \]

\[ \sigma(\vec{p}) d\vec{p} = \sigma_0 [N_{\text{cas}}(\vec{p}) + N_{\text{pr}(\vec{p})} + N_{\text{eq}}(\vec{p})] d\vec{p} \]
Simulating Accelerator Radiation Environments
Fourth International Workshop (SARE4)
Hyatt Regency, Knoxville, TN, September 13-16, 1998

Improved Cascade-Exciton Model of Nuclear Reactions

Stepan G. NIASHNIK and Arnold J. SIERK
T-2, Theoretical Division
Los Alamos National Laboratory
Los Alamos, NM, 87545
Comparison between the main assumptions of the CEM97, Bertini, and ISABEL INC models

<table>
<thead>
<tr>
<th>Method</th>
<th>CEM97</th>
<th>Bertini</th>
<th>ISABEL</th>
</tr>
</thead>
<tbody>
<tr>
<td>INC stage</td>
<td>Improved Dubna INC</td>
<td>INC + EQ or INC + PE + EQ</td>
<td>the same</td>
</tr>
<tr>
<td>Monte Carlo technique</td>
<td>“spacelike”</td>
<td>the same</td>
<td>timelike</td>
</tr>
<tr>
<td>Nuclear density distribution</td>
<td>$\rho(r) = \rho_0 / \left( \exp\left(\frac{r-c}{a}\right) + 1 \right)$</td>
<td>the same</td>
<td>the same</td>
</tr>
<tr>
<td></td>
<td>$c = 1.07 A^{1/3}$ fm, $a = 0.545$ fm</td>
<td>the same</td>
<td>the same</td>
</tr>
<tr>
<td></td>
<td>$\rho(r) = \alpha_i \rho_0(r); i = 1, \ldots, 3$</td>
<td>$\alpha_1 = 0.9, \alpha_2 = 0.2, \alpha_3 = 0.01$</td>
<td>$\alpha_1 = 0.9, \alpha_2 = 0.2, \alpha_3 = 0.01$</td>
</tr>
<tr>
<td>Nucleon potential</td>
<td>$V_N = T_F + B_N$</td>
<td>the same</td>
<td>Nucleon kinetic energy ($T_N$)</td>
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<tr>
<td>Pion potential</td>
<td>$V_\pi = 25$ MeV</td>
<td>$V_T = T_N$</td>
<td>nucleon energy from mass table;</td>
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<tr>
<td>Mean binding nucleon energy</td>
<td>$B_N \approx 7$ MeV</td>
<td>the same</td>
<td>the same value is used throughout the calculation</td>
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<tr>
<td>Elementary cross sections</td>
<td>new, CEM97, last update March 1999</td>
<td>standard Bertini INC (old)</td>
<td>standard ISABEL (old)</td>
</tr>
<tr>
<td>A + A interactions</td>
<td>not considered</td>
<td>the same</td>
<td>allowed</td>
</tr>
<tr>
<td>$\gamma A$ interactions</td>
<td>may be considered</td>
<td>not considered</td>
<td>not considered</td>
</tr>
<tr>
<td>Condition for passing from the INC stage</td>
<td>$P = \max\left{ W_{mod.} - W_{exp.} \right} \right</td>
<td><em>{W</em>{exp.}} P = 0.3</td>
<td>cutoff energy $\approx 7$ MeV</td>
</tr>
<tr>
<td>Nuclear density depletion</td>
<td>not considered</td>
<td>the same</td>
<td>considered</td>
</tr>
<tr>
<td>PE stage</td>
<td>Improved MEM (CEM97)</td>
<td>MPM (LAHET) model</td>
<td>the same</td>
</tr>
<tr>
<td>EQ stage</td>
<td>CEM97 model for $n, p, d, t, ^3He, ^4He$</td>
<td>Dreiser model for $n, p, d, t, ^3He, ^4He$</td>
<td>the same</td>
</tr>
<tr>
<td></td>
<td>emission ($\gamma$) + fission ($\gamma$)</td>
<td>emission ($\gamma$) + fission ($\gamma$)</td>
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<tr>
<td>Level density</td>
<td>CEM97 models for $a = a(Z,N,E')$</td>
<td>LAHET models for $a = a(Z,N,E')$</td>
<td>the same</td>
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<td>Multifragmentation of light nuclei</td>
<td>Fermi breakup as in LAHET</td>
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<td></td>
<td>RAL fission fragmentation</td>
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1. Condition for passing from the INC stage

$P = \max\left\{ W_{mod.} - W_{exp.} \right\} \right|_{W_{exp.}} P = 0.3$
Comparison between the main assumptions of the MEM (CEM97) and MPM (LAHET)

<table>
<thead>
<tr>
<th>Master equation; computation method</th>
<th>MEM (CEM97), differs from MPM; Monte Carlo</th>
<th>MPM (LAHET), differs from MEM the same</th>
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<td>( \Delta n = +2, 0, -2 )</td>
<td>only ( \Delta n = +2 )</td>
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<tr>
<td>Matrix elements for nuclear transitions</td>
<td>MEM algorithm: (</td>
<td>M</td>
</tr>
<tr>
<td>Pauli correction term</td>
<td>( A = (p^2 + h^2 + p - h)/4 - h/2 )</td>
<td>( A = E_{Pauli} - [p(p + 1) + h(h + 1)]/4g_0 )</td>
</tr>
<tr>
<td>Multiple particle emission</td>
<td>allowed, no limitation</td>
<td>the same</td>
</tr>
<tr>
<td>Type of particle considered</td>
<td>n, p, d, t, (^3\text{He}, ^4\text{He})</td>
<td>the same</td>
</tr>
<tr>
<td>Level density parameter, ( g = 6a(A, Z, E^*)/\pi^2 )</td>
<td>CEM97 parameterization (+ 9 CEM95 options)</td>
<td>Ignatyuk (from GNASH)</td>
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<td>Dostrovsky</td>
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<td>forward picked, CEM algorithm: either by Master equation or from kinematics</td>
<td>initially, isotropic; Kalbach parameterization may be applied later</td>
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</table>
$\text{fission of } ^{197}\text{Au by neutrons}$

- staples' data
- CEM95, $af/an = 1.10$
- CEM97, $af/an = 1.10$; thermally damped ground-state shell correction

Fission Cross Section (mb)

Neutron Lab Kinetic Energy (MeV)
Cross Sections of Spallation Residues Produced in 1\(A\) GeV\(^{208}\)Pb on Proton Reactions

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(Received 11 February 2000)

Spallation residues produced in 1 GeV per nucleon \(^{208}\)Pb on proton reactions have been studied using the Fragment Separator facility at GSI. Isotopic production cross sections of elements from \(^{61}\)Pm to \(^{82}\)Pb have been measured down to 0.1 mb with a high accuracy. The recoil kinetic energies of the produced fragments were also determined. The obtained cross sections agree with most of the few existing gamma-spectroscopic data. The data are compared with different intranuclear-cascade and evaporation-fission models. Drastic deviations were found for a standard code used in technical applications.

PACS numbers: 25.40.Sc, 24.10.–i, 25.70.Mn, 29.25.Dz

Spallation reactions have recently captured an increasing interest due to their technical applications as intense neutron sources for accelerator-driven subcritical reactors [1] or spallation neutron sources [2]. The design of an accelerator-driven system (ADS) requires precise knowledge of nuclide production cross sections in order to be able to predict the amount of radioactive isotopes produced inside the spallation target. Indeed, short-lived isotopes may be responsible for maintenance problems and long-lived ones will increase the long term radiotoxicity of the system. Recoil kinetic energies of the fragments are important for studies of radiation damages in the structure materials or in the case of a solid target. Data concerning lead are particularly important since in most of the ADS concepts actually discussed, lead or lead-bismuth alloy is considered as the preferred material of the spallation target.

The present experiment, using inverse kinematics, is able to supply the identification of all the isotopes produced in spallation reactions and information on their recoil velocity. Moreover, the data represent a crucial benchmark for the existing spallation models used in the ADS technology. The precision of these models to estimate residue production cross sections is still far from the performance required for technical applications, as it was shown in Ref. [3]. This can be mostly ascribed to the lack of complete distributions of all produced isotopes to constrain the models. The available data were generally obtained by chemistry or gamma spectroscopy [4–6] which give access mostly to cumulative yields produced after long chains of decaying isotopes.

In this Letter, we report on complete isotopical production cross sections for heavy fragments produced in spallation of \(^{208}\)Pb on proton at 1\(A\) GeV, down to 0.1 mb with a high precision. The kinematic properties of the residues are also studied. The cross sections of lighter isotopes produced by fission will be presented in a forthcoming publication.

The experimental method and the analysis procedure have been developed and applied in previous experiments [7–9]. The primary beam of 1\(A\) GeV \(^{208}\)Pb was delivered by the heavy-ion synchrotron SIS at GSI, Darmstadt. The proton target was composed of 87.3 mg/cm\(^2\) liquid hydrogen [10] enclosed between thin titanium foils of a total thickness of 36 mg/cm\(^2\). The primary-beam intensity was continuously monitored by a beam-intensity monitor (SEETRAM) based on secondary-electron emission. In order to subtract the contribution of the target windows from the measured reaction rate, measurements were repeated with the empty target. Heavy residues produced in the target were all strongly forward focused due to the inverse reaction kinematics. They were identified using the Fragment Separator (FRS) [11].

The FRS is a two-stage magnetic spectrometer with a dispersive intermediate image plane (S\(_2\)) and an achromatic final image plane (S\(_4\)) with momentum acceptance of 3\% and angular acceptance of 14.4 mrad around the beam axis. Two position-sensitive plastic scintillators placed at S\(_2\) and S\(_4\), respectively, provided the magnetic-rigidity \(Bp\) and time-of-flight measurements, which allowed to determine the mass-over-charge ratio of the particles. In the analysis, totally stripped residues were considered only. In the case of residues with the highest nuclear charges (above \(^{65}\)Tb) an achromatic degrader (5.3 to 5.9 g/cm\(^2\) of aluminum) was placed at S\(_2\) to obtain a better \(Z\) resolution. The elements below terbium were identified from an energy-loss measurement in an ionization chamber (MUSIC). The velocity of the identified residue was determined at S\(_2\) from the \(Bp\) value and transformed into the frame of the beam in the middle of the target taking into account the appropriate energy loss. About 100
FIG. 2. Isotopic production cross-sections of elements between $Z=82$ and 61, in the reaction of 1-Å GeV $^{208}$Pb on hydrogen, versus neutron number. Stable (resp. radioactive) isotopes are marked by open (resp. full) triangles. Gamma-spectroscopy data regarding shielded isotopes from [6] are plotted as open circles. The solid, dashed and dotted curves were calculated with the Cugnon-Schmidt [20,21], Bertini [16]-Dresner [18,19] and Isabel [17]-Dresner models, respectively.

cross-section is the sum of the production of the ground and the isomeric states. The data agree within their error bars, except for the isotope with the lowest cross-section.

to the fact that the prediction of the neutron-proton evaporation competition in the Dresner code is not satisfying. The magnitude of the measured and calculated
FIG. 3. Mass distribution (upper panel) and recoil kinetic energy (bottom panel) of the residues produced in 1·A GeV $^{208}$Pb on hydrogen reactions (triangles) versus mass number, compared with the Cugnon-Schmidt (solid line), Bertini-Dresner (dashed line) and Isabel-Dresner (dotted line) models. The dash-dotted line shows the recoil kinetic energies expected from the Morrissey systematics [23].

The velocity distribution of each residue was also determined, from which it was possible to infer information about the recoil kinetic energy in the projectile system. In the bottom part of Fig. 3, the...
1 GeV p on Pb208

residual nucleus production

Cross section (mb)

Mass number
Mass yields in Pb-208 irradiated with 1GeV protons

![Graph showing mass yields and kinetic energy distributions for Pb-208 irradiation with 1GeV protons.](image-url)
Product isotopic distributions in $^{208}\text{Pb}+1\text{GeV}$: GSI+ZSR+ITEP+LAHET(isabel)
Product isotopic distributions in $^{208}$Pb+1GeV: GSI+ZSR+ITEP+LAHET (bertini)
Product isotopic distributions in $^{208}$Pb+1GeV: GSI+ZSR+ITEP+INUCL
Product isotopic distributions in $^{208}$Pb+1GeV: GSI+ZSR+ITEP+CASCADE

Product mass
Product isotopic distributions in $^{208}\text{Pb}+1\text{GeV}$: GSI+ZSR+ITEP+CASCADE
Product isotopic distributions in $^{208}\text{Pb}+1\text{GeV}$: GSI+ZSR+ITEP+YIELDX

![Graphs showing product isotopic distributions](image)

- CRS [mbarn] vs. Product mass for various elements.
Isotopic distributions of the products in Pb-208+1GeV protons: GSI+ITEP+Codes
Isotopic distributions of the products in Pb-208+1GeV protons: GSI+ITEP+Codes

![Graph showing isotopic distributions with labels for different isotopes and curves for CEM97, CEM97mod, and CEM2k.]
Isotopic distributions of the products in Pb-208+1GeV protons: GSI+ITEP+Codes
Product isotopic distributions in $^{208}\text{Pb}+1\text{GeV}$: GSI+ZSR+ITEP+CEM2k

CRS [mbarn] vs. Product mass
Products in Pb-208 irradiated with 1GeV protons

Cross section [mb]

Product isotopes and their cross sections are plotted against a logarithmic scale. The chart includes various symbols and colors representing different models and experimental data. The isotopes are listed along the bottom axis, and the cross sections are depicted along the vertical axis.
Further work

- fission cross sections
- fission fragment A-, Z-, T-, E*- , L-distributions
- inverse cross sections
- complex particle and fragment emission
- where to stop evaporation, at
  \[ A = 4 \text{ (most models)}, \]
  \[ A = 18 \text{ (Botvina, Shmakov, Uzhinsky'95)}, \]
  \[ A = 20 \text{ (Schmidt'98)}, \]
  \[ A = 28 \text{ (Furihata'00)}, \]
  or even further?
- criteria for transaction from INC to PE and from PE to EV
- do we need to use in-medium elementary cross sections, and where to take them from?
- reliable optical potential for all particles, not only nucleons
- ...