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Title: AN EXAMPLE OF A MONTE CARLO CODE APPLIED TO THE MODELING OF COMPLEX SYSTEMS

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TOPIC 2
Monte Carlo Transport from Zero to 200 MeV

AN EXAMPLE OF A MONTE CARLO CODE APPLIED TO THE MODELING OF COMPLEX SYSTEMS

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1. Introduction

Current interest in the use of accelerators for nuclear applications is high in the United States, Japan and Europe. Table 1 contains a listing of the current and planned high power accelerators operating with spallation targets in the 'intermediate' energy range (~up to 2 GeV)[1].

Facility	Proton Beam Energy (MeV)	Average Current	Beam Power (MW)	Target
Currently Operating Facilities				
SINQ, PSI, Switzerland	590	1.8 mAmp	1.062	Zircaloy Rods
LANSCE Area A, LASREF Los Alamos	800	1 mAmp	0.800	Typically tungsten targets
LEDA, APT, Los Alamos, USA	6.7	100 mAmps	0.670	Low Energy Demonstration Accelerator
ISIS, Rutherford Appleton Lab, UK	800	200 μAmps	0.16	Tantalum plate target
Lujan Center, LANSCE, Los Alamos, USA	800	100 μAmps	0.08	Split tungsten target
WNR, LANSCE Los Alamos USA	800	30 μAmps	0.003	Tungsten target
IPNS, Argonne National Lab, USA	500	15 μAmps	0.008	Depleted Uranium plate target
Japanese Spallation Neutron Source	500	5 μAmps	0.0025	Depleted Uranium plate target
Planned Facilities				
APT, Savannah River, USA	1030	100 mAmps	103.0	Clad tungsten cylinder targets
ATW, USA	1000	30 mAmps	30.0	Lead-bismuth, other options
SNS, Oak Ridge, USA	1000	2 mAmps	2.0	Liquid mercury
European Spallation Source	1334	3.7 mAmps	5.0	Liquid mercury

Table 1 Current and Planned Accelerators with Spallation Targets

There are two major uses for such facilities; as spallation neutron sources for basic neutron scattering research (SINQ, ISIS, Lujan, WNR, IPNS, JSNS, SNS, ESS), and as

[1] Note the simple rule that beam power in MWatts is given by multiplying beam energy in MeV by average current in Amps.

nuclear facilities primarily for isotope production and destruction (LASREF, LEDA/APT, ATW). The latter are generally 'continuous' proton beams, without any pulsed structure. The former almost always include pulse capability to facilitate the timing of neutron scattering events.

The applications of 'continuous' beam proton accelerators envisioned today include :

- Production of isotopes for research and medical uses
- Transmutation of nuclear wastes
- Power production, particularly as a biproduct of other applications
- Generation of tritium for nuclear stockpile use

Such applications have created a need for improved computer simulation tools, particularly in the Monte Carlo area. The demand for deterministic methods is present, and will increase as criticality issues are examined in waste transmutation applications. However many existing codes can already handle the necessary calculations. The primary need in deterministic methods is for multigroup libraries expanded in upper energy range. In addition, certain questions remained unsolved in deterministic methods, particularly involving charged particle transport. Until these issues are adquately addressed, heavy reliance will continue to be placed on Monte Carlo methods in the design and analysis of accelerator-based nuclear systems. Despite the need for additional computational time, Monte Carlo methods provide the best possible modeling for detailed structure of target geometry and shielding. Coupled with transmutation codes such as CINDER or ORIGIN, the full neutronics history of a system may be obtained. The use of intermediate energy Monte Carlo codes is also not confined to high power accelerator systems. A listing of current applications for the MCNPX code is given in Table 2.

Application	Number of Groups
Design of Spallation Targets	18
Waste Treatment, Energy Ampification	19
High altitude aircraft dosimetry	7
Spacecraft shielding	18
Radiography	8
Materials Studies	4
Accelerator Health Physics	25
Neutrino Target Design	3
Experimental Physics detectors	7
Other Detector development	11
Cross section & physics model development	11
Conventional reactor physics	1
Medical	24
Irradiation facilities	2
Radioactive beam facilities	1

Table 2 Number of MCNPX Beta Test Groups by Code application

For intermediate energy, high power accelerator applications, uses of Monte Carlo codes are numerous, and form the basis for validation through benchmarking and other activities. Examples include :

- Neutronics/particle performance of target/blanket systems
- Heat loading from energy deposition and decay heat
- Mateirals and corrosion damage parameters
- Shielding design
- Dosimetry
- Air and groundwater activation
- Criticality studies
- Transmutation effectiveness
- Safety source terms

Processes specific high energy interaction are illustrated in Figure 1. Above the tabular limits, interaction and transport physics in current Monte Carlo codes is handled by physics routines which calculate needed quantities as the transport occurs. The fundamental nuclear interaction process is handled by intranuclear cascade (INC) models, supplemented with pre-equilibrium physics. The residual nucleus goes through an evaporation process, or breakup for light nuclei. High energy fission routines further supplement the suite of available models. These features are discussed in the section 2, as implemented into the MCNPX[2] Monte Carlo code.

The MCNPX code development project involves the formal extension of MCNP4B[3] to all particles and all energies. It has become an important tool for the analysis of nuclear applications for accelerators, currently with ~500 users internationally. In section 3 we discuss the code development, new features, and specific benchmarking activities.

2 Elements of Intermediate and High Energy Monte Carlo Codes

A number of models typically go into high energy Monte Carlo code systems, and Table 3 gives a summary of options available in the MCNPX code. These, along with general particle transport physics, are discussed in the following sections.

2.1 Intranuclear Cascade Models (INC)

The concept of an Intranuclear Cascade (INC) model is quite old, intuitively simple, and as a practical matter, unrivaled for speed of computation. A particle incident on a nucleus will interact with individual nucleons, with final states defined by a set of fundamental free particle-particle cross sections. Above ~200 MeV, the production of pions becomes important, and these are generated via isobar formation and decay. In some models, such resonances can themselves interact, however this adds considerably to calculational time. In general, INC methods do not include correlation effects in the nuclear medium, although newer models are investigating this.

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[2] L. S. Waters, ed., 'MCNPX User's Manual, version 2.1.5', Los Alamos National Laboratory LA-UR 99-6058, November 14, 1999.

[3] J. F. Briesmeister, ed., 'MCNP™ – A General Monte Carlo N-Particle Transport Code', Los Alamos National Laboratory Report LA-12625-M, Version 4B (March 1997).

The nucleus is considered to be a cold, free gas of nucleons confined within a potential that describes nucleon binding energies, and the nuclear density as a function of radius. Fermi motion of the nucleons is considered in the elementary collisions. The quantum effects of Pauli blocking are taken into account. These features are fairly generic to all INC models, with differences usually limited to nuclear potential descriptions, particularly in the paramertization of density distributions. Standard Wood-Saxon potentials are used, although the actual profile is often modeled as a series of steps rather than as a continuous function to minimize computational time. Nuclear density depletion as the cascade proceeds is usually not modeled.

A key element of INC model interactions is the decision to terminate nucleon-nucleon interactions. Experimental data show that evaporation phases typically begin at $\sim 10^{-16}$ seconds. Some INC codes keep track of all interaction times to ensure that the INC phase stops at a reasonable time. Such 'timelike' codes typically fit experimental data to determine the optimum cutoff time, however this parameter can be adjusted by the user. In 'spacelike' codes, the INC phase is terminated by tracking the energy of the interaction, terminating when this falls below the mean nucleon binding energy plus code-dependent cutoff energy parameter of the oder of several MeV.

MCNPX offers three choices of INC models, the Bertini[4], ISABEL and CEM[5]. The Bertini model is incorporated into MCNPX through the LAHET Code System[6] implementation of the HETC Monte Carlo code developed at Oak Ridge National Laboratory[7]. The ISABEL model was included in MCNPX directly from the LAHET Code System[8]. ISABEL is derived from the VEGAS INC code[9]. It has the capability of treating nucleus-nucleus interactions as well as particle-nucleus interactions, although this capability has not been fully tested in the MCNPX implementation.

2.4 Multistage Pre-equilibrium Models (MPM)

Subsequent de-excitation of the residual nucleus after the INC phase may optionally employ a multistage, multistep preequilibrium exciton model, or MPM[10]. The MPM is invoked at the completion of the INC, with an initial particle-hole configuration and excitation energy determined by the outcome of the cascade. At each stage in the MPM, the excited nucleus may emit a neutron, proton, deuteron, triton, ^{3}He or alpha; alternatively, the nuclear configuration may evolve toward an equilibrium exciton number by increasing the exciton number by one particle-hole pair. The MPM terminates upon reaching the equilibrium

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[4] H. W. Bertini, Phys. Rev 131, (1963) pp 1801
H. W. Bertini, Phys. Rev. 188 (1969) pp 1711

[5] S. G. Mashnik and V. D. Toneev, 'Modex – The Program for Calculation of the Energy Spectra of Particles Emitted in the Reactions of Pre-equilibrium and Equilibrium Statistical Decays ', JINR P4-8417, Dubna, 1974.

[6] R. E. Prael and H. Lichtenstein, 'User Guide to LCS : The LAHET Code System', Los Alamos National Laboratory Report LA-UR-89-3014, revised. (September 15, 1989)

[7] Radiation Shielding Information Center, 'HETC Monte Carlo High-Energy Nucleon-Meson Transport Code', Report CCC-178, Oak Ridge National Laboratory (August 1977).

[8] Y. Yariv and Z. Fraenkel, Phys Rev C 20 (1979) pp 2227
Y. Yariv and Z. Fraenkel, Phys Rev C 24 (1981) pp 488

[9] K. Chen, et. al., Phys. Rev, 166 (1968) p949

[10] R. E. Prael and M. Bozoian, 'Adaptation of the Multistage Pre-equilibrium Model for the Monte Carlo Method (1)', Los Alamos National Laboratory Report, LA-UR-88-3238, September 1998.

exciton number, at which point an evaporation or Fermi-Breakup model is then applied to the residual nucleus with the remaining excitation energy.

In the LAHET/Bertini model, the inverse reaction cross sections are represented by the parameterization of Chatterjee. The potentials from which the inverse reaction cross sections are obtained are those selected by Kalbach [11] for the PRECO-D2 code.

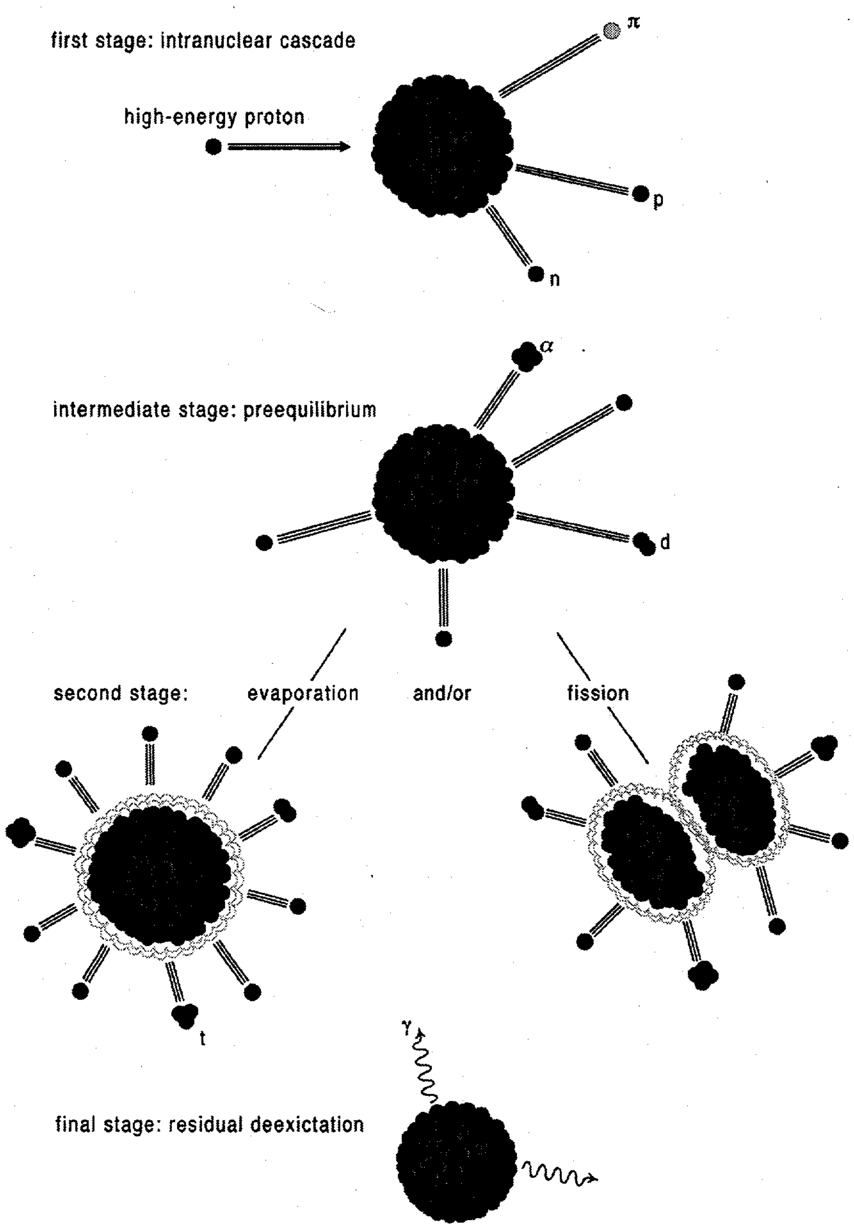

Figure 1 Processes involved in high energy particle/nucleus interactions

[11] PRECO-D2 : Program for Calculating Preequilibrium and Direct Reaction Double Differential Cross Sections, LA-10248-MS, Los Alamos National Laboratory, 1985.

Physics Process	Bertini	ISABEL	CEM
Method	INC+EQ or INC+PE+EQ	INC+EQ or INC+PE+EQ	INC + PE + EQ
Intranuclear Cascade Model	Bertini INC	ISABEL INC	improved Dubna INC
Monte Carlo Technique	"spacelike"	"timelike", but uses energy cutoff for termination of INC	"spacelike"
Nuclear Density Distribution	$\rho(r)=\rho_0\{\exp[(r-c)/a]+1\}$ $c=1.07A^{1/3}$ fm a=0.545 fm $\rho(r)=\alpha_i\rho(0)$; i = 1,...,3 $a_1=0.9$, $a_2=0.2$ $a_3=0.01$	$\rho(r)=\rho_0\{\exp[(r-c)/a]+1\}$ $c=1.07A^{1/3}$ fm a=0.545 fm $\rho(r)=\alpha_i\rho(0)$; i=1,...,16	$\rho(r)=\rho_0\{\exp[(r-c)/a]+1\}$ $c=1.07A^{1/3}$ fm a=0.545 fm $\rho_n(r)/\rho_p(r) = N/Z$ $\rho(r)=\alpha_i\rho(0)$; i = 1,...,7 $a_1=0.95$, $a_2=0.8$ $a_3=0.5$ $a_4=0.2$ $a_5=0.1$ $a_6=0.05$ $a_7=0.01$
Nucleon Potential	$V_N = T_F + B_N$	Nucleon kinetic energy (T_N) dependent potential $V_N=V_i(1-T_N/T_{max})$	$V_N = T_F + B_N$
Pion Potential	$V_\pi = V_N$	$V_\pi = 0$	$V_\pi = 25$ MeV
Mean Nucleon Binding Energy	$B_N \sim 7$ MeV	initial B_N from mass table; the same value is used throughout the calculation	$B_N \sim 7$ MeV
Elementary Cross Sections	standard BERTINI INC (old)	standard ISABEL (old)	new CEM97, last update March 1999
A + A interactions	not considered	allowed	not considered
γA photonuclear interactions	not considered	not considered	Under development
Condition for passing from the INC stage	For each cascade nucleon check to see if energy is below Woods-Saxon potential + cutoff energy of 7 MeV	different cutoff energies for p and n, as in VEGAS code	W_{mod} (the imaginary part of the optical potential) is compared to experimental data. $P=\|(W_{mod}-W_{exp})/W_{exp}\|$ If P<30%, continue INC
Nuclear density depletion	not considered	considered	not considered
Pre-equilibrium stage	MPM (LAHET) model	MPM (LAHET) model	Improved MEM (CEM97)
Equilibrium stage	Dresner model for n, p, d, t, ^{3}He, ^{4}He emission (+ fission) (+ γ)	Dresner model for n, p, d, t, ^{3}He, ^{4}He emission (+ fission) (+ γ)	CEM97 model for n, p, d, t, ^{3}He, ^{4}He emission (+ fission) (+ γ)
Level density	Three LAHET models for A=a(Z,N,E*)	Three LAHET models for A=a(Z,N,E*)	CEM97 model for a=a(Z,N,E*)
Multifragmentation of light nuclei	Fermi breakup as in LAHET	Fermi breakup as in LAHET	Fermi breakup as in LAHET
Fission models	ORNL or RAL models	ORNL or RAL models	CEM model for sf, RAL fission fragmentation

Table 3 Summary of Physics Options in MCNPX

When the ISABEL intranuclear cascade model is invoked, it is possible to determine explicitly the particle-hole state of the residual nucleus since a count of the valid excitations from the Fermi sea (and the filling of existing holes) is provided. To define the initial conditions for the MPM, the number of particle-hole pairs is reduced by one for each intranuclear collision for which both exiting nucleons are below the top of the nuclear potential well. This method is the only option implemented in MCNX to link the MPM with the ISABEL INC.

In adapting the MPM to the Bertini INC, it has not been possible yet to extract the same detailed information from the intranuclear cascade history. Consequently, the algorithm which defines the interface between the Bertini INC and the MPM is a rather crude approximation, intended to permit initial evaluation of the MPM but open to further improvement. In this case, the initial condition for the MPM is one particle-hole pair beyond the minimum particle-hole configuration allowed by the outcome of the INC. The adaptive algorithm used with ISABEL is quite effective. However, given the initial condition algorithm used with the Bertini INC, the user has a choice of invoking the MPM in one of three optional modes, (or not at all):

1. The MPM continues from the final state of the INC with the initial condition defined as above ("normal MPM").
2. The INC is used only to determine that an interaction has occurred and the MPM proceeds from the compound nucleus formed by the absorption of the incident particle ("pure MPM").
3. A random selection is made of one of the above modes at each collision with a probability $P = \min[E_1/E_c, 1.0]$ of choosing the "pure MPM" mode where E_c is the incident energy and E_1=25 MeV ("hybrid MPM").

The addition of preequilibrium models to INC codes is essential to obtaining the proper angular distribution of secondary particles, as shown in Figure 2.

2.5 Evaporation and Breakup Models

MCNPX, when used with the Bertini or ISABEL options, employs the Dresner evaporation model, based on work orginally due to Weisskopf[12]. After the INC/MPM stage, residual nuclei are in highly excited states, and energy is disappated by evaporation of n, p, d, t, ^{3}He and α particles. The probability $p(\varepsilon)$ that an excited nucleus will emit a particle x with kinetic energy ε is proportional to :

$$(2S_x+1)m_x\varepsilon\sigma_{cx}(\varepsilon)\omega(E)$$

Where S_x and m_x are the spin and mass of particle x, σ_{cx} is the cross section for formation of the compound nucleus in the inverse reaction (bombarding the residual nucleus with particles of energy ε), E is the excitation of the residual nucleus, and $\omega(E)$ is the density of levels of the residual nucleus at excitation E. A discussion of level density options is given in section 2.7 below.

Although the Dresner model can emit 19 different particles from a nucleus, only those with Z up to 2 are implemented in MCNPX. The probability of emission of a particle is given by

[12] V. F. Weisskopf, Phys. Rev. 52, 295 (1937)

$$R_x = (2S+1)m_x \int_{k_x V_x}^{U-Q_x-\delta} \varepsilon\sigma_{cx}(\varepsilon)\omega(U-Q_x-\delta-\varepsilon)d\varepsilon$$

Q_x is the binding energy of the particle in the nucleus, and k_x are taken from inverse cross section parameterizations for each particle. V_x is the Columb barrier, and U is the initial excitation energy. These integrals have been solved analytically for different particles :

$$R_{neutron} = A^{2/3}\alpha[I_1(S)+\beta I_o(S)]e^s$$

$$R_{charged} = 1/2(2S_x+1)m_x(1+C_x)A^{2/3}I_1(S)e^S$$

$$S = 2\sqrt{a(U-k_xV_xQ_x-\delta)}$$

$$I_o(S) = (2a)^{-1}(S-1+e^{-S})$$

$$I_1(S) = (8a2)^{-1}(2S^2-6S+6+e^{-S}[S^2-6])$$

Where the parameters A, α, β, a, δ, k and V all refer to the residual nucleus. The value of k_x is 0 for neutrons. Rx is set to zero if $U \geq k_xV_x+Q_x+\delta$. Next R_x is summed over all emission particles, and the history is terminated if the value is zero, and the relative probablity of emission for each type calculated. The actual selection of a particular particle to evaporate is determined by random selection. The energy spectrum of an evaporated particle is :

$$N(\varepsilon_x)d\varepsilon_x = T_x^{-2}(\varepsilon_x - k_xV_x)e^{-(\varepsilon_x-k_xV_x)/T_x}d\varepsilon_x$$

With $k_xV_x \leq \varepsilon_x <$ infinity. T_x is a constant depending on the level density of the residual nucleus and equal to half the average value of $\varepsilon_x - k_xV_x$.

The Fermi-Breakup model[13] has replaced the evaporation model for the disintegration of light nuclei. It treats the deexcitation process as a sequence of simultaneous breakups of the excited nucleus into two or more products, each of which may be a stable or unstable nucleus or nucleon. Any unstable product nucleus is subject to subsequent breakup. The probability for a given breakup channel is primarily determined from the available phase space, with probabilities for two-body channels modified by Coulomb barrier, angular momentum, and isospin factors. The model is applied only for residual nuclei with A≤17, replacing the evaporation model for these nuclei. In the LAHET/MCNPX implementation, only two- and three-body breakup channels are considered; it is an abbreviated form of a more extensive implementation of the Fermi-Breakup model, with up to 7-body simultaneous breakup, used previously for cross section calculations on light nuclei[14].

2.6 High Energy Fission Models

Two models for fission induced by high-energy interactions are included in MCNPX, The ORNL Model[15], and the Rutherford Appleton Laboratory (RAL) model[16]. The RAL model

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[13] D. J. Brenner, R. E. Prael, J. F. Dicello and M. Zaider, 'Improved Calculations of Energy Deposition from Fast Neutrons', in Proceedings, Fourth Symposium on Neutron Dosimetry, EUR-7448, Munich-Neuherberg (1981).

[14] D. J. Brenner and R. E. Prael, 'Calculated Differential Secondary-particle Production Cross Sections after Nonelastic Neutron Interactions with Carbon and Oxygen between 10 and 60 MeV,' Atomic and Nuclear Data Tables 41, 71-130 (1989).

[15] J. Barish, T. A. Gabriel, F. S. Alsmiller and R. G. Alsmiller, Jr., 'HETFIS High-Energy Nucleon-Meson Transport Code with Fission', Oak Ridge National Laboratory Reprot ORNL-TM-7882 (July 1981)

allows fission for Z≥71 and is the default in MCNPX. It is actually two models, one for actinide and one for subactinide fission.The ORNL model covers fission only for actinides.

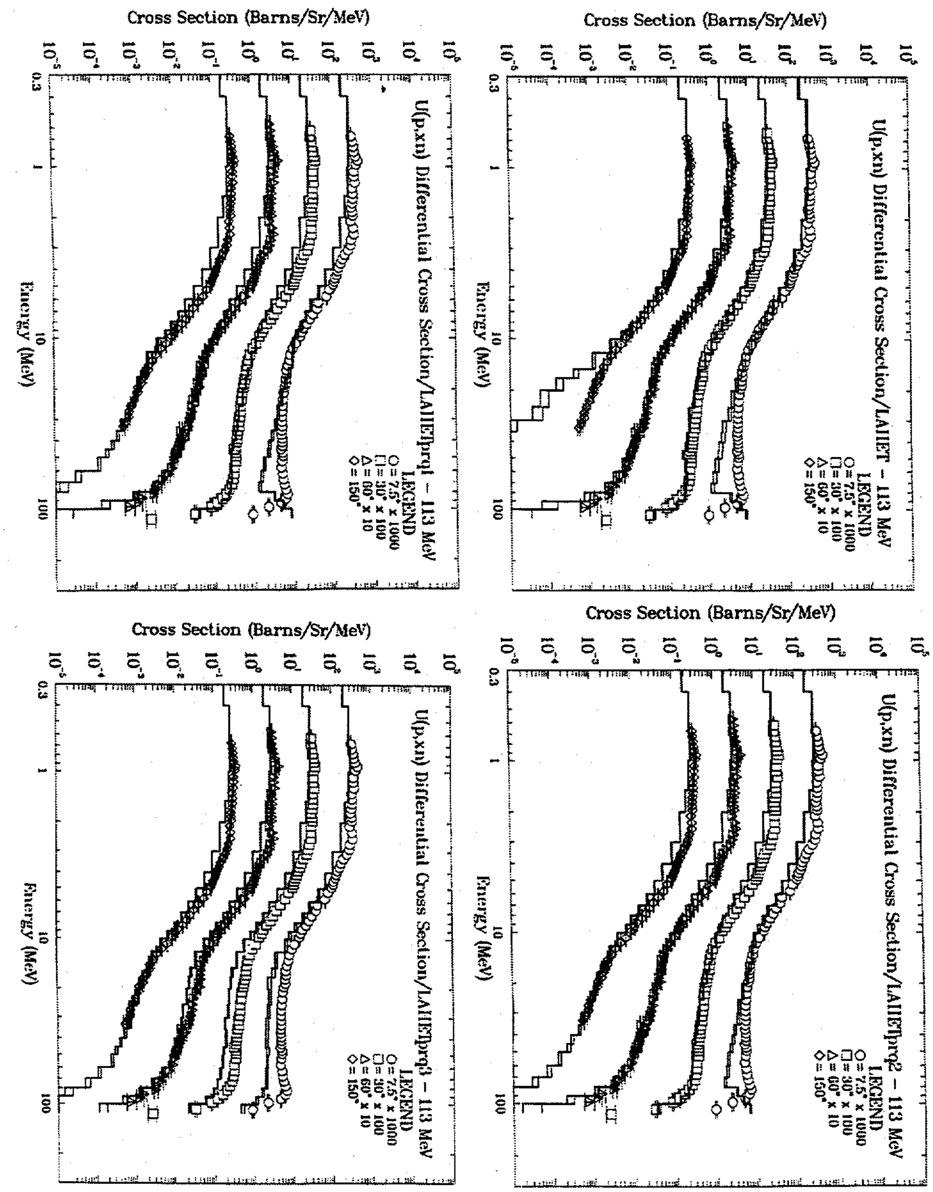

Figure 2. Bertini Model INC Calculations without Pre-equilibrium, and with the 3 MCNPX Pre-equilibrium options. Calculation is the straight line, data are symbols.

The subactinide fission routines of the RAL model produce cross sections which tend to be low compared to the most recent data, and use of pre-equilibrium models further reduce these values. This is strong indication that improvements in subactnide fission models are warranted.

[16] F. Atchison, 'Spallation and Fission in Heavy Metal Nuclei under Medium Eenrgy Proton Bombardment', in Targets for Neutron Beam Spallation Sources, Jul-Conf-34, Kernforschungsanlage Julich GmbH (January, 1980).

2.7 Level Densities

As the excitation energy of a nucleus increases, excited level states get closer together in energy. Methods of statistical mechanics and thermodynamics have long been used to describe the structure of a highly excited nucleus. At large excitation energy E, the density of excited levels 1/D, where D is the average distance between levels, is of the form:

$$C = ae^{2(a\sqrt{E})}$$

where C and a are parameters which are functions of the mass number and must be empirically adjusted. Generally C is evaluated from the observed level density at low excitation (E~1 MeV), and a is adjusted to represent the spacing of levels found from the resonance capture of slow neutrons (E~6 to 8 MeV). Users of intermediate energy simulations codes have long known that results are highly sensitive to how the 'a' parameter is set. Three options for level density parameters are offered by the Bertini and ISABEL codes.

Ignatyuk model: The default evaluation of the level density parameter a uses the energy dependent formulation of Ignatyuk as implemented in GNASH with the provision that:

$$\lim_{E \to 0} a(E) = a_0$$

where E is the excitation energy and a_0 is the Gilbert-Cameron-Cook level density parameter. Both low and high excitation limits are illustrated in the top of Figure 3.

Julich model: A second model is the mass dependent model developed for the Julich version of HETC (DRE81). In MCNPX it is applied as originally formulated, independent of energy, but could be used as the low-excitation limit in the Ignatyuk model.

HETC model: The third option is the mass and isospin dependent model originally used in the evaporation model of HETC (DRE81):

$$a = a(1 + y_0(A - 2Z)^2) / b_0$$

where the default values $b_0 = 8.0$ and $y_0 = 1.5$ may be changed by the user. Figure 3 illustrates the different options.

2.8 Nuclear data

Starting in 1996, the APT project undertook the extension of standard nuclear data evaluations to 150 MeV for a number of elements of interest to the plant design. At the same time proton evaluations were also developed, and a program of photonuclear library development is underway. Since that time other programs have contributed funding for other elements. For example, the Spallation Neutron Source (SNS) program has funded the development of mercury evaluations in order to design their liquid mercury target. Programs involved in accelerator transmutation are working on actinide libraries. MCNPX version 2.1.5 can take full advantage of all features of the extended neutron libraries, and 2.1.6 will add proton and photonuclear libraries. In addition, work is underway to produce libraries of certain light ion reactions. The 150 MeV neutron libraries are released with MCNPX version 2.1.5 under the name LA150N. The entire set of 150 MeV neutron, proton and photonuclear libraries can be used with MCNPX version 2.1.6, and will be released under the names LA150N, LA150H and LA150U. As the generation of these libraries is well covered elsewhere in this lecture series, we will defer to the notes of Dr. Arjan Koning for futher information.

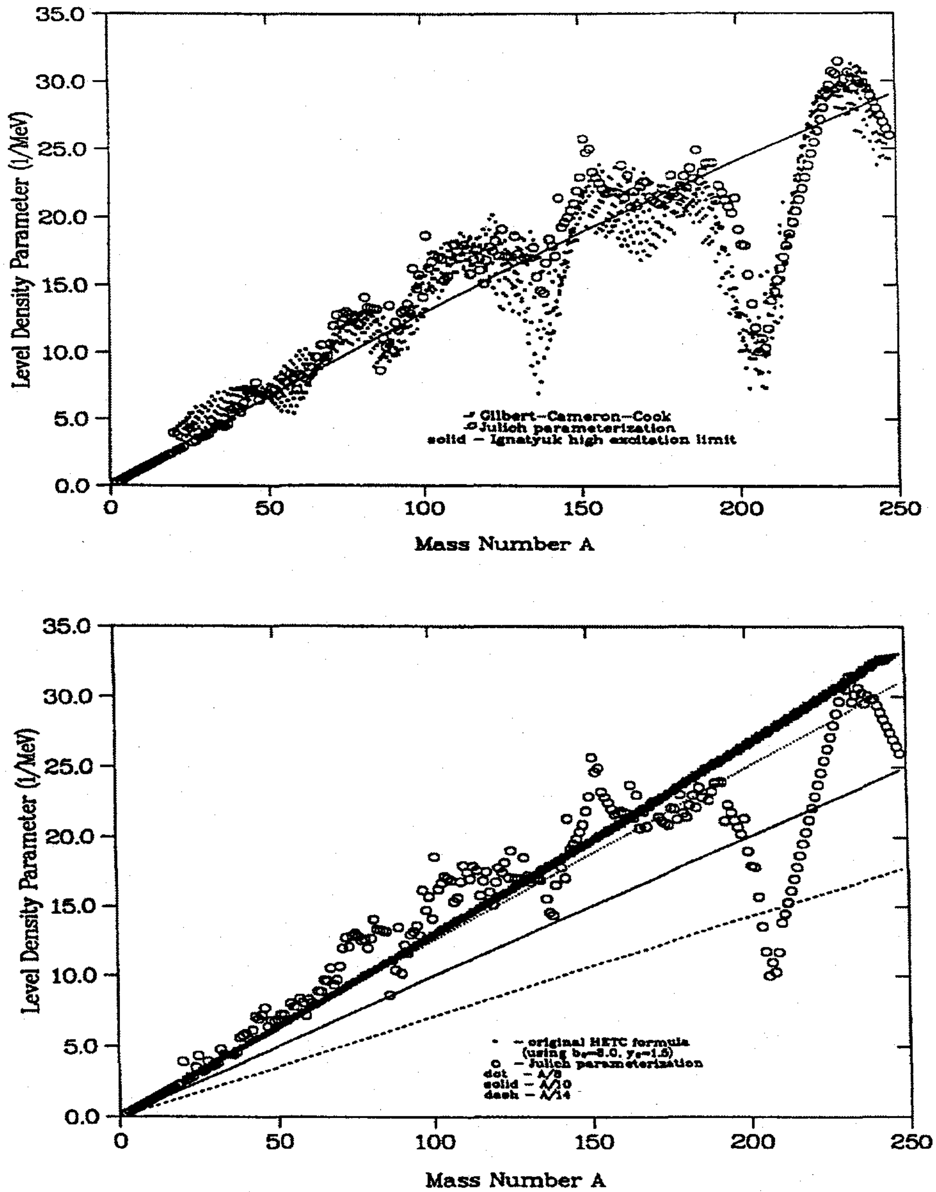

Figure 3 Level Density Options. Top : Low and high-excitation limits of the Ignatyuk model, compared with the Julich parameterization. Bottom : Original HETC formulation

Additional information is needed by Monte Carlo codes in the form of total, elastic and reaction cross sections above the tabular region. New global optical model potentials for nucleon-nucleus scattering up to 2 GeV are underway, using both Schrodinger and Dirace formalisms[17]. In support of this work, new cross section measurements have recently been made at the Los Alamos WNR facility for neutron total cross sections, and at the Brookhaven AGS for proton reaction cross sections. Figure 4 summarizes some of the recently released neutron cross sections.

2.9 Energy Straggling and Multiple Scattering

[17] D. G. Madland and A. J. Sierk, 'Development of Global Medium-Energy Nucleon-Nucleus Optical Model Potentials', International Conference on Nuclear Data for Science and Technology, Trieste, Italy, May 19-24, 1997.

MCNPX, like MCNP4B, uses a sophisticated implementation of the Landau theory for electrons, as described in the MCNP4B manual. For heavy charged particles, the assumptions of the Landau theory breakdown, and the more complex Vavilov theory[18]must be used. At low energies and large step sizes, the Vavilov distribution approaches a Gaussian. At very high energies, or small step sizes (and for electrons in almost all circumstances), the Vavilov distribution approaches a Landau distribution.

The module implemented in MCNPX to represent the Vavilov model does attempt to account for the Gaussian and Landau limits, when step sizes and energies are appropriate. Further improvements in this module are expected in future versions of MCNPX.

The full Goudsmit-Saunderson model of multiple scattering for electrons as implemented in MCNP4B/MCNPX is described in the MCNP4B manual. In MCNPX version 2.1.5, a small-angle Coulomb scattering treatment has been implemented for heavy charged particles. We use a Gaussian model based on a theory presented by Rossi. In the original theory, both angular deflections and small spatial displacements were accounted for. Since the complex geometric system of MCNPX does not yet accommodate transverse displacements in charged-particle substeps, we use only the part of the theory that addresses the angular deflection. In several test cases, this slight approximation has been found to have negligible effect on the results.

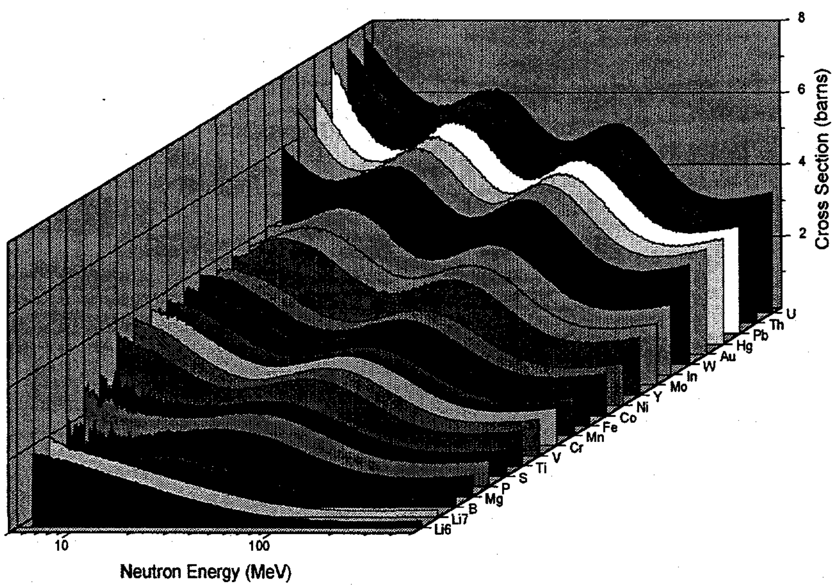

Figure 4 Neutron Total Cross Sections

[18] P. V. Vavilov, 'Ionization Losses of High-Energy Heavy Particles', Sofiet Physics JETP 5, No. 5 (1957) 749.

3 The MCNPX Code Project

The MCNPX code project was started in 1994, and involves the formal extension of MCNP4B to all particles and all energies. Additional tallies and varience reduction techniques specific to accelerator applications have also been added. 42 ENDF neutron data libraries have been extended in energy to 150 MeV (100 MeV for Be-9), and a similar set of proton libraries has been formulated. 12 photonuclear libraries have also been evaluated, and physics modules put in place above the photonuclear tabular limit. Physics models are available from the LAHET Code System, and also from the CEM code. Information on the code and beta test program can be found at http://www.mcnpx.gov

3.1 Software Management for Nuclear Applications

Given the potential of MCNPX for nuclear applications, software management concerns have been paramount from the beginning of this project. Most high intensity applications will be classified as Nuclear Category 2 facilities, necessitating an extraordinary amount of software quality assurance. MCNPX follows the formality of the Capability Maturity Model (CMM) process, which designates 5 levels of software process maturity (one being lowest, five being highest). This system is mandated for Department of Energy facilities, according to DOE order. MCNPX is striving for a level 3 ranking, currently we are close to 2. The categorization is based on the following 18 process areas:

- **Requirements Management** : Establish customer requirements
- **Software Project Planning** : Establish reasonable plans for code development
- **Software Tracking and Oversight** : Establish action plans in case of deviations
- **Software Subcontract Management** : Select and manage qualified subcontractors
- **Software Quality Assurance** : Tracking and feedback into the development process
- **Software Configuration Management** : Estabilish and maintain product integrity throughout the life cycle
- **Organization Process Focus** : Establish responsibilities for software process activities
- **Organization Process Definition** : Establish and maintain software process assets
- **Training Program** : Develop skills and knowledge of developers and users
- **Integrated Software Management** : Integrate software engineering and management activities
- **Software Product Engineering** : Consistently perform a well defined engineering process integrating all software engineering activities
- **Intergroup Coordination** : Establish means for software engineering group to interact with other engineering groups
- **Peer Reviews** : Remove defects from the product early and efficiently
- **Quantitative Process Management** : Measure progress quantitatively
- **Software Quality Management** : Develop a quantitative understanding of the quality of the product to achieve specific qualitygoals
- **Defect Prevention** : Identify causes of defects and prevent them from reoccuring
- **Technology Change Management** : Integrate new tools into the organization as needed
- **Process Change Management** : Continually improve the software process in the organization

3.2 Modifications from MCNP4b

The first change that was implemented into MCNPX was the expansion of the number of particles allowed for transport. Table 4 gives the complete list of currently trackable particles.

IPT	Name of Particle	Symbol	Mass (MeV)	Low Kinetic Energy Cutoff (MeV)	Mean Lifetime (seconds)
1	neutron (n)	n	939.56563	0.0	887.0
1	anti-neutron (n)	n	939.56563	0.0	887.0
2	photon (g)	p	0.0	0.001	huge
3	electron (e-)	e	0.511008	0.001	huge
3	positron (e+)	e	0.511008	0.001	huge
4	muon- (μ-)	|	105.658389	0.11261	2.19703 x 10-6
4	anti-muon- (μ+)	|	105.658389	0.11261	2.19703 x 10-6
6	electron neutrino (νe)	u	0.0	0.0	huge
6	anti-electron neutrino	u	0.0	0.0	huge
9	proton (p)	h	938.27231	1.0	huge
9	anti-proton (p)	h	938.27231	1.0	huge
20	pion+ (π+)	\	139.56995	0.14875	2.6033 x 10-8
20	pion- (π-)	\	139.56995	0.14875	2.6033 x 10-8
21	neutral pion (π0)	z	134.9764	0.0	8.4 x 10-17
22	kaon+ (K+)	k	493.677	0.52614	1.2386 x 10-8
22	kaon- (K-)	k	493.677	0.52614	1.2386 x 10-8
23	K0 short	%	497.672	0.000001	0.8927 x 10-10
24	K0 long	^	497.672	0.000001	5.17 x 10-8
31	deuteron	d	1875.627	2.0	huge
32	triton	t	2808.951	3.0	12.3 years
33	Helium-3	s	2808.421	3.0	huge
34	Helium-4 (a)	a	3727.418	4.0	huge

Table 4 Transportable Particles in MCNPX

Although other particles can be produced in high energy interactions, these are basically unstable and will be decayed to a set of trackable particles. These are shown in Table 5. The Pi0 is a special case ; it is always decayed immediately to two gammas. Tables in the MCNP output file formats were adapted to include the new particle list.

In order to simulate interactions above the tabular limits, physics models from the LAHET and CEM codes were included. Current code development involves adding the capability to switch between table based and physics based transport at an arbitrary energy. This 'Mix and Match' problem involves a recoding of nuclear data structures in the main code, and is currently a high priority in code development.

MCNPX is dedicated to a modular approach, with the maintenance of a core code which interfaces with separate modules. Currently we are investigating the CORBA object oriented programming protocol to handle these interfaces. An interface document is being written, and MCNPX version 3.0 will be the first to implement the new format. This will also allow us to easily update to MCNP4C features.

MCNP4B input files are compatible with MCNPX, as are all MCNP4B libraries. A few MCNP4C library features will be ignored in MCNPX until the 4C update is complete.

IPT	Name of Particle	Symbol	Mass (MeV	Low Kinetic Energy Cutoff (MeV)	Mean Lifetime (seconds)
Leptons					
5	tau- (t-)	*	1777.1	1.894	2.92 x 10-5
7	muon neutrino (nm)	v	0.0	0.0	huge
8	tau neutrino (nt)	w	0.0	0.0	huge
Baryons					
10	lambda0 (L0)	l	1115.684	1.0	2.632 x 10-2
11	sigma+ (S+)	+	1189.37	1.2676	7.99 x 10-3
12	sigma- (S-)	-	1197.436	1.2676	1.479 x 10-2
13	cascade (X0)	x	1314.9	1.0	2.9 x 10-2
14	cascade- (X-)	y	1321.32	1.4082	1.639 x 10-2
15	omega- (W-)	o	1672.45	1.7825	8.22 x 10-3
16	lambdac+ (Lc+)	c	2285.0	2.4353	2.06 x 10-5
17	cascadec+ (Xc+)	!	2465.1	2.6273	3.5 x 10-5
18	cascadec0 (Xc0)	?	2470.3	1.0	9.8 x 10-6
19	lambdab0 (Lb0)	r	5641	1.0	1.07 x 10-4
Mesons					
25	D+	G	1869.3	1.9923	1.05 x 10-4
26	D0	d	1864.5	1.0	4.15 x 10-5
27	Ds+	f	1968.5	2.098	4.67 x 10-5
28	B+	j	5278.7	5.626	1.54 x 10-4
29	B0	b	5279.0	1.0	1.5 x 10-4
30	Bs0	q	5375.	1.0	1.34 x 10-4

Table 6 Non-transportable Particles (decayed upon production)

3.3 New Tallies

The technique which has become known as the "Mesh Tally" has become very widely used in accelerator applications. The use of this method grew out of research with codes such as LCS, GEANT, FLUKA, CALOR, and MARS at the Superconducting Super Collider in 1993. Some form of this method is currently in standard use in most high-energy Monte Carlo codes.

The Mesh Tally is a method of graphically displaying particle flux, dose, or other quantities on a rectangular, cylindrical or spherical grid overlaid on top of the standard problem geometry. Particles are tracked through the independent mesh as part of the regular transport problem, and the contents of each mesh cell written to a file at the end of the problem. This file can be converted into a number of standard formats suitable for reading by various graphical analysis packages. The conversion program, gridconv, is supplied as part of the overall MCNPX package. This is an overview of neutron fluence in a spallation target system. Analysis of this data is limited only by the capabilities of the graphical program being used.

A capability has also been added to MCNPX to allow the code to generate simulated radiography images as one would expect to see from an X-ray or pinhole projection of an object containing the particle source.This allows the recording of both the direct (source) image as well as that due to background (scatter). This tool is an invaluable aid to the problem of image enhancement, or extracting the source image from a background of clutter.

MCNPX includes two types of image capability; the pinhole image projection and the transmitted image projection.

Special forms of the F6 energy deposition tally have been added to MCNPX to take account of higher energy, charged particle processes. Two forms are available. The first is the original F6 :P form which uses heating numbers as contained in data tables for photons or neutrons. This tally has now been expanded to include all particles, and track ionization, nuclear recoil energy and the energy from untracked secondary particles also included. A special form, +F6 :n,p has also been added to give energy deposition from all particles.

3.4 New Variance Reduction Techniques

The unique characteristics of Intranuclear Cascade processes, particularly the copious production of low energy neutrons from a single incident particle, means that special variance reduction techniques must be designed. Leading Particle or Secondary Particle biassing techniques bias the cascade toward the particle of interest. Secondary particle biasing has been introduced into the MCNPX code for two main reasons.

- It allows splitting of secondary particles from high-energy cascades in the energy range of interest.
- It allows the user to roulette the large number of particles in energy ranges that are of no interest to the problem.

This technique is especially useful in deep penetration problems starting with very high-energy particles where the very large number of low-energy secondary particles have little or no chance of contributing to the answer. On the other hand, one needs all of the high-energy particles that one can get.

MCNPX version 2.1.5 has been upgraded to allow the user to control the numbers of secondary particles as a function of energy and primary particle interaction.

3.6 Benchmarking Activities for MCNPX

The APT benchmarking program for MCNPX is extensive, with activities ongoing in the following areas :

- Production of neutrons from spallation targets (Saturne/Sunnyside waterbath measurements
- Production of tritium in He-3 gas
- Decay heat from a tungsten sample using compensating calorimetry
- Decay heat from a complex system in LANSCE Area A
- Energy deposition in a semi-prototypic APT target with incident protons
- Energy deposition in a water phantom with neutrons
- Radionuclide production in thick targets with incident proton beams
- Numerous studies from existing literature, particularly in deep penetration shielding problems.

As an illustration, a measurement of energy deposition has been performed at the WNR continuous neutron source facility at LANSCE. This is a benchmark in support of the calculation of high energy fluence-to-dose conversion coeficients. Figure 5 shows the water phantom target, Figure 6 shows the WNR measured spectra under several different colimation systems, and Figure 7 shows some recent MCNPX code comparisons.

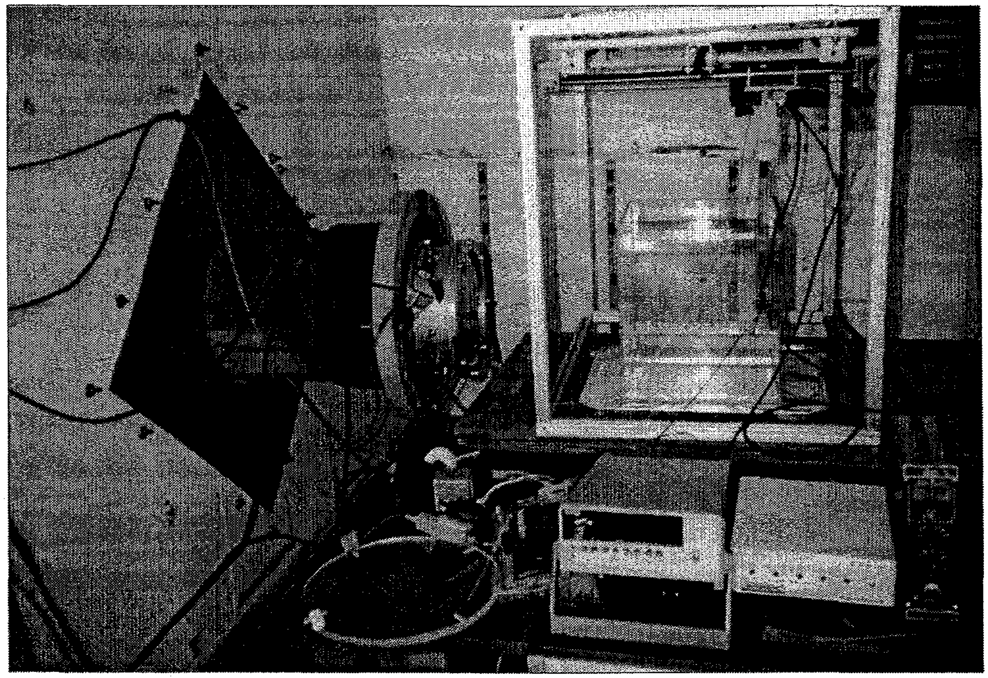

Figure 5 Water phantom setup

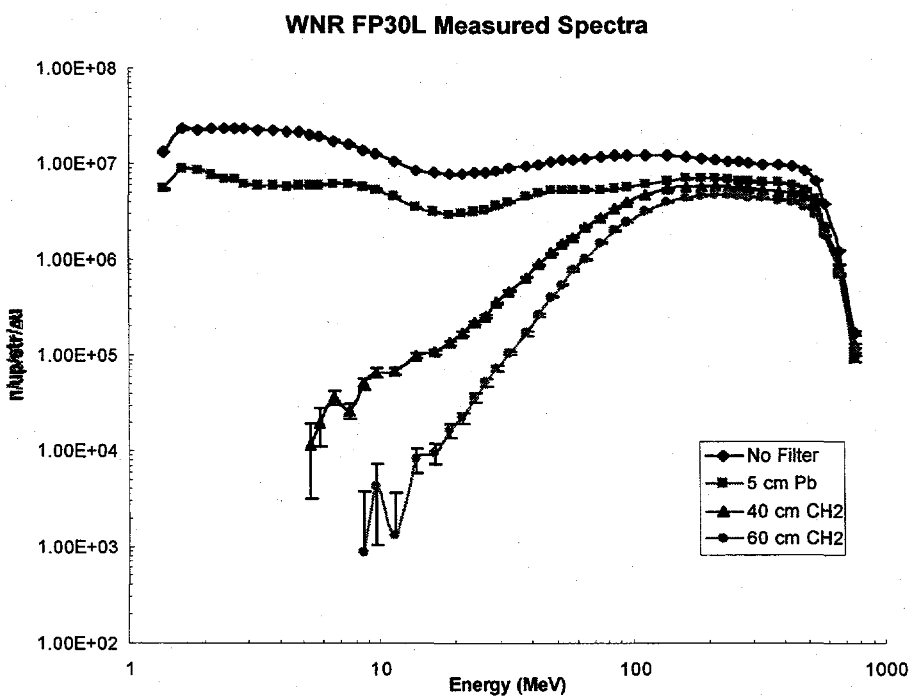

Figure 6 WNR Spectra in the 30 degree left beamline, using several different collimators to filter out low energy neutron and photon components

Figure 7 Comparison of MCNPX and energy deposited in the phantom for an unfiltered beam. This simulation depends heavily on the accurate modeling of the target to get photon and low energy neutron components correct.