Nuclear Modeling for Applications in Medical Radiation Therapy and Accelerator-Driven Technologies

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Nuclear Modeling for Applications in Medical Radiation Therapy and Accelerator-Driven Technologies

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An understanding of the interactions of neutrons and protons below a few hundred MeV with nuclei is important for a number of applications. In this paper, two new applications are discussed: radiation transport calculations of energy deposition in fast neutron and proton cancer radiotherapy to optimize the dose given to a tumor; and intermediate-energy proton accelerators which are currently being designed for a range of applications including the destruction of long-lived radioactive nuclear waste. We describe nuclear theory calculations of direct, preequilibrium, and compound nucleus reaction mechanisms important for the modeling of these systems.

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I. INTRODUCTION

The interaction of a nucleon projectile with a target nucleus involves a number of different reaction mechanisms such as direct, preequilibrium, and compound nucleus emission processes. Theories for describing preequilibrium reactions, in particular, have received a great deal of attention over the last few decades because of interest in describing a many-body system in a non-equilibrium state [1]. These theories describe the interaction as a multistep scattering processes, and include semiclassical exciton and hybrid models and quantum mechanical formulations [1]. The energy and momentum brought in by the projectile are shared with an increasing number of target nucleons via nucleon-nucleon collisions, and particle emission from the early stages of the reaction gives the typically high-energy and forward-peaked continuum preequilibrium spectrum. The multistep theory of Feshbach, Kerman, and Koonin (FKK) [2], in particular, has been widely applied due to the fact that it can generally account for many features of the experimental data, including angular distributions, while being fairly straightforward to apply computationally [3].

It is not the purpose of this paper, however, to review recent developments in preequilibrium theories. Such a review can be found in the excellent book by Gadioli and Hodgson [1]. Instead, here we wish to discuss two applications where an accurate modeling of preequilibrium processes is important: radiation transport simulations of fast neutron and proton cancer radiation therapy; and proposed high-current proton-accelerators, with energies of the order of 1 GeV, for applications which include the transmutation of long-lived radioactive waste into shorter-lived products, energy production, and the production of tritium. These projects involve collaborations between national laboratories, universities, research hospitals, and industrial partners.

In both applications it is essential to understand how a medium-energy projectile nucleon interacts with matter, how it deposits its energy, and how the secondary particles are transported through matter. Preequilibrium processes are critically important since they govern the extent of high-energy particle production, and account for much of the energy deposition. Applications and nuclear theory developments are linked by nuclear data evaluators, who attempt to provide the most accurate information concerning nuclear reaction processes using input from experimental measurements and nuclear theory predictions. Since the number of laboratories for measuring nuclear cross sections is shrinking throughout the world, with decreasing budgets, the role of nuclear theory for guiding evaluations is assuming an increasing importance.

This paper is organized as follows. Sec. II gives an overview of the nuclear physics needed to predict the interaction of low-medium energy nucleons with nuclei, and some of the computer codes that can be used to calculate cross sections. Sec. III discusses nuclear data for calculations of energy deposition in fast neutron and proton radiation therapy, concentrating on work being performed in the Lawrence Livermore National Laboratory PEREGRINE project. Sec. IV describes modeling developments required for an accurate description, and optimization, of accelerators that are currently being designed in the USA, Europe, and Japan.
II. NUCLEAR THEORY FOR APPLICATIONS

Most applications of nuclear reaction physics ultimately involve performing radiation transport analyses of a system, that is, determining how radiation (neutrons, protons, electrons, photons, etc.) interacts and passes through matter. Such analyses frequently involve determining the fluxes and energy spectra of the transported radiation, determining the energy deposited, calculating the production of radioactive products (activation), and determining material damage from the knock-on recoil of atoms.

Radiation transport codes tend to make use of microscopic nuclear cross sections in one of two fundamentally-different ways: either by calculating them "on the fly" on an event-by-event basis; or by "looking up" a pre-evaluated cross section from an evaluated nuclear database. An example of the former type is the Los Alamos LAHET code system [4], which has been widely used to simulate accelerator target configurations. A well known example of the latter is the Los Alamos MCNP transport code, which typically reads microscopic cross sections from evaluated databases such as ENDF, or ENDL (the Livermore databases). However, until recently virtually all the evaluated databases exist only below 20 MeV, since they were originally developed for nuclear fission and fusion applications.

There are a number of advantages to using evaluated nuclear data files rather than "on-the-fly" nuclear reaction calculations within the transport code: (1) the most accurate possible nuclear models and theories can be used to generate the data; (2) the data can be carefully checked against existing measurements, and integral benchmarks (such as comparing predictions against kerma factors - see the next section) can be performed to validate the libraries; and (3) the results of model calculations can be modified to better agree with experimental measurements where they exist. A further reason for using evaluated data libraries is the following. The nuclear models used within transport codes such as LAHET, which calculate cross sections internally using intranuclear cascade methods (INC), tend not to be accurate at energies below about 150 MeV. Below 150 MeV the underlying physical assumptions of the INC theory (e.g. that the mean-free path in the nucleus is large compared to the nucleon wavelength) are not well satisfied. For this reason, there are significant improvements that can be made in the modeling of a system if evaluated databases are used up to about 150 MeV incident energy. Above this energy, the gains in using evaluated databases are probably not large.

Therefore, a number of laboratories are currently working on the production of evaluated nuclear databases up to a few hundred MeV, and the next two sections describe the requirements of nuclear databases for two different applications. In the remainder of this section, we summarize the nuclear models that may be used to produce these databases.

As a means of introducing the various nuclear reaction models that are important, Fig. 1 shows a calculated angle-integrated neutron spectrum in the channel-energy frame (produced with the LANL/LLNL code FKK-GNASH [5]), for 80 MeV neutrons.
on carbon [6]. At the highest emission energies the importance of neutron inelastic scattering to the 2+ (4.4 MeV) and 3- (9.6 MeV) states in carbon is evident. The nuclear reaction mechanisms which contribute are as follows [6,7]:

- At the highest emission energies, direct reactions to the low-lying states are dominant. These can be calculated with DWBA or coupled-channel optical models.

- The long hard tail in the spectrum is due to preequilibrium processes (both primary, and multiple - where more than one fast particle is emitted). These can be calculated with quantum mechanical theories such as FKK, or the semiclassical exciton or hybrid models.

- At low energies, compound nucleus emission accounts for the large evaporation-type spectrum. This can be calculated with Hauser-Feshbach or Weisskopf-Ewing theories, or Fermi break-up [8] for light nuclei.

\[
\begin{align*}
\text{Fig. 1. Calculated 80 MeV } & ^{12}\text{C}(n, xn) \text{ angle-integrated inclusive emission spectrum, with contributions from primary and multiple preequilibrium emission.} \\
\end{align*}
\]

A number of deterministic nuclear modeling codes have been developed to calculate nuclear cross sections up to 100-200 MeV, which can be used to generate nuclear data libraries. These include:

- GNASH, a Los Alamos code [7] which uses Hauser-Feshbach theory to calculate sequential decay processes in an open-ended chain of decays, conserving spin and parity. Low-lying nuclear levels are included, above which a statistical level density is used. Preequilibrium processes are calculated using the semiclassical exciton model, and direct reaction cross sections may be included.
- FKK-GNASH, a Los Alamos - Livermore code [5] similar to the above, but which uses the quantum mechanical FKK theory for preequilibrium processes.
- MINGUS, a ECN-Petten code [10] which uses FKK theory for preequilibrium emission and Weisskopf-Ewing theory for evaporation.

III. MEDICAL RADIOTHERAPY APPLICATIONS

The Lawrence Livermore National Laboratory PEREGRINE project is developing an all-particle Monte Carlo transport code for calculating and optimizing absorbed dose in cancer radiotherapy [11]. This code transports neutrons, photons and charged particles in a fully coupled manner, and can be used for simulating the effects of radiation beams on the dose delivered to a patient. The transport is performed through a three-dimensional mesh obtained from a CT-scan of the patient, and the calculated dose distributions can be used to optimize the dose delivered to a tumor.

The PEREGRINE code can be used for simulations of all the major types of radiotherapy: electrons, photons, neutrons, and protons. However, it is fast neutron therapy which requires the most detailed understanding of nuclear reaction processes. Nuclear reactions are also of importance in proton therapy, though most of the energy deposition by protons comes from electronic “dE/dx” slowing down, and nuclear reactions here mainly influence the depletion of the primary proton beam.

Most modern fast neutron therapy facilities use a $^9$Be$(p, n)$ source reaction, which produces a broad spectrum of neutrons with energies up to 70 MeV. In a recent review of the status of nuclear data for use in neutron therapy, White et al.[12] emphasized that with the exception of hydrogen, sufficiently accurate nuclear data does not yet exist in this energy range to allow neutron therapy to reach its full potential. Since “standard man” consists (by mass) of hydrogen (10%), carbon (18%), nitrogen (3%), and oxygen (65%), and various trace elements (4%), an accurate understanding of neutron nuclear reactions on these light nuclei (particularly carbon and oxygen) is essential. One of the main mechanisms for energy deposition in neutron therapy is elastic scattering of neutrons by hydrogen, which dominates the absorbed dose until high energies (about 60 MeV), where reactions on oxygen become more important. Fortunately elastic scattering on hydrogen is known very well at these energies.

We have produced evaluated cross section libraries up to 100 MeV for neutrons on biological elements, for use in the PEREGRINE code. Since the experimental data for neutron reactions on biologically-important elements is limited, we have based our evaluations mainly on nuclear theory and model calculations, benchmarked to the measurements where they exist. To do this, we have developed and applied the FKK-GNASH modeling code [7, 5], which uses Hauser-Feshbach theory for equilibrium decay, Feshbach-Kerman-Koonin (FKK) [2] theory for preequilibrium emission,
includes corrections for direct processes. Elastic scattering is included via optical model calculations.

Generally it is rather difficult to accurately calculate inelastic cross sections on light nuclei, since statistical assumptions that the theories make do not hold well when the spacing of nuclear levels is large. However, we have found that our model calculations describe experimental data surprisingly well. In part this is because our implementation of Hauser-Feshbach theory uses experimental nuclear level schemes for low excitation energies where a statistical level-density model is not applicable. It is also due to the fact that even in nuclei such as carbon and oxygen the density of nuclear states above about 10 MeV excitation energy becomes large enough for non-statistical effects to become small.

As examples of our results, in Fig. 2 we show the evaluated cross section for \( ^{16}\text{O}(n, xp) \) at 40 MeV compared measurements from UC-Davis [13]. The importance of high-energy protons from preequilibrium processes is evident. In Fig. 3 we show our 60 MeV \( ^{12}\text{C}(n, x\alpha) \) evaluation compared with data from UC-Davis and Louvain-la-Neuve. Again, the calculations are seen to describe the data well. The particularly large alpha production cross section seen is because the tight binding of alpha particles results in carbon fragmentation often producing alpha particles, in many cases through the \( 3\alpha \) break-up mechanism.

![Graph](image_url)

**Fig. 2.** Calculated angle-integrated 40 MeV \( ^{16}\text{O}(n, xp) \) spectrum compared with experimental data [13].
Accurately predicting charged-particle emission spectra is particularly important since the charged ejectiles have a small range and deposit their kinetic energy as heat (and breaking molecular DNA bonds killing cells). The absorbed dose in the body is therefore closely related to the product of the production cross sections and average energies of the charged particles, and this quantity is known as the kerma (an acronym for *kinetic energy released in matter*). An important test of our evaluated libraries is, therefore, that they should account for measured kerma factors. In Figs. 4 and 5 we show the kerma, derived from our microscopic cross section databases, compared with measurements for carbon and oxygen. The agreement seen between calculation and experiment provides an important benchmarking of our evaluations.
Fig. 4. Total carbon kerma factor derived from cross section calculations compared with experimental data (see Ref. [6] for references to the data).

Fig. 5. Total oxygen kerma factor derived from cross section calculations compared with experimental data [15–18].
As an example of the content of the LLNL medical nuclear databases, we show in Fig. 6 the double differential cross sections for neutrons, protons, deuterons, and alpha particles following the interaction of 50 MeV neutrons with carbon. In each figure we show the emission spectra at angles every ten degrees, with the highest values being at 0-degrees, and the lowest being at 180-degrees. These pictures allow one to clearly see the trends in the cross sections. The importance of preequilibrium reactions is evident, due to the strong forward-peaking of the spectra, especially at the high outgoing energies. At low energies the forward-peaking is due to the fact that these cross sections are in the laboratory frame of reference. The structure that is seen is due to the inclusion of low-lying discrete states in the calculation, and the variation of the structure with angle shows the kinematical effects when the calculations are transformed into the lab frame.

Fig. 6. Double-differential evaluated emission spectra in the laboratory frame following 50 MeV neutrons on carbon.

The PEREGRINE code will be particularly useful for predicting absorbed dose to a tumor which is close to a critical structure, such as the spinal-column, or an optic nerve. In such cases, it is essential that the energy deposited occurs in the treatment volume, and that a minimum dose is given to the surrounding structure. The strength of using PEREGRINE to optimize the clinical radiation beam configurations here is that the Monte Carlo method automatically takes into account inhomogeneities in
the body, unlike most conventional methods used in treatment planning systems.

As an example of the energy deposition in the body calculated by PEREGRINE, we show in Fig. 7 the calculated dose when a 150 MeV proton beam, and a 70 MeV neutron beam, are incident on the body. This is, of course, just an example, and a patient would not be treated in this way! But the example shows the different ways in which energy is deposited in the body by neutrons and protons, as well as the effects of inhomogeneities. The picture shows a CT-scan through the chest. The variations in energy deposition were originally shown as rainbow colors, but on a grey scale these variations are harder to see. On the left hand side is a 150 MeV proton beam and on the right a 70 MeV neutron beam. In the case of neutrons the energy deposition decreases with depth, whereas with protons most energy deposition occurs at the end of the proton range, giving the Bragg peak. The inhomogeneity effects of the lower density in the lung can be clearly seen.

Fig. 7. PEREGRINE calculations of absorbed dose following neutron and proton radiation beams on the chest. A CT-scan slice is shown, with colors superimposed designating the different dose regions.

Further details of this work can be found in Ref. [6,11].
IV. ACCELERATORS FOR WASTE-BURNING

There is currently a great deal of interest in the U.S.A., Europe, and Japan, to develop approx. 1 GeV proton accelerators which can be used as a spallation neutron source [19]. Such accelerators have a number of applications with include the transmutation (or “burning”) of long-lived radioactive waste into shorter-lived products, energy production (in a fundamentally sub-critical system), and tritium production. Spallation neutrons are also of interest in condensed matter studies. Production of neutrons in this manner has some significant advantages over using a reactor – primarily because the system is not close to critical, and so is inherently safer, and the environmental impact is significantly better since fission products are not produced.

The basic general design of these systems is a high energy proton beam that is incident on a stopping-length target, typically made of a high-Z material such as tungsten or lead. Nuclear collisions result in the production of secondary neutrons and protons, which may then further undergo nuclear collisions. In a system which is large enough to thermalize the nucleons and prevent leakage of high-energy particles, one obtains typically 1 thermal neutron for each 40 MeV incident proton energy - in other words, for a 1 GeV beam, about 25 thermal neutrons. Approximately one quarter of the incident kinetic energy can be converted into mass (i.e., separation energy for neutron production), and the rest of the energy is ultimately converted into heat. One of the key design parameters is how many thermal neutrons are produced for each incident proton, i.e. \((n/p)\), since this quantity drives the overall efficiency (and cost) of the machine. This quantity, in turn, can be predicted by nuclear model codes.

Nuclear model codes such as LAHET [4] have played an important role in the design of spallation targets. For instance, at Los Alamos the code has been extensively used to optimize the design of the targets and blankets. However, design uncertainties in the accelerator system can be significantly reduced by extending the evaluated transport nuclear data libraries up to 150 MeV, for implementation in radiation transport calculations.

At present the evaluated databases used by the Los Alamos Monte Carlo transport code, MCNP, extend up to 20 MeV, and above this energy model calculations are performed with LAHET. However, in the region from 20-150 MeV, deterministic preequilibrium/equilibrium statistical model codes have been shown to predict cross sections more accurately [20]. An accurate description of nuclear reactions from 20-150 MeV will be particularly important for predicting \((n/p)\) since \((n,xn)\) and \((p,xn)\) reactions contribute significantly in this energy range. In Fig. 8 we show experimental nonelastic cross sections for neutrons on lead compared with results from both LAHET and FKK-GNASH model calculations. The FKK-GNASH results were obtained from a coupled-channels optical model, whereas the LAHET result is obtained from intranuclear cascade methods. While the LAHET results are seen to describe the data well at higher energies, it is evident that the FKK-GNASH calculations describe
the data significantly better below 150 MeV. This example demonstrates that use of evaluated data libraries up to 150 MeV (generated using both experimental data and model calculations with a code such as FKK-GNASH) will improve the modeling of the target/blanket of an accelerator system.

![Graph showing reaction cross section for 208Pb+n](image)

**Fig. 8.** Calculated reaction (nonelastic) cross section for 208Pb+n compared with experimental data. The optical potential used by the FKK-GNASH code is described in Ref. [21].

The recent intermediate-energy code intercomparison by Blann et al. for the Nuclear Energy Agency of the OECD [20] compared the predictions of a range of modeling codes with experimental data for proton reactions on lead and zirconium. One conclusion from this intercomparison was that deterministic codes such as FKK-GNASH, GNASH, and ALICE describe measurements more accurately below 200 MeV than do intranuclear cascade codes. As an example of one of the reactions considered in the intercomparison, Fig. 9. shows FKK-GNASH calculations of the inclusive 160 MeV 90Zr(p, xn) reaction, compared with data of Scobel et al. [22]. Different contributions from FKK-theory multistep direct (MSD) preequilibrium stages are shown, for both primary particle emission and multiple preequilibrium emission (where a second fast particle is emitted). It is evident that one and two-step scattering dominates the contribution to high-energy neutron emission, and that higher-order scatterings become important at low emission energies. The full calculation describes the data well.

In addition to predicting (n/p), nuclear theory calculations, and data evaluation, are also important for modeling other processes in the system. Induced-radioactivity
can be calculated by predicting the build-up of radioactive product nuclides in nuclear reactions. Heating estimates can be calculated, as can material damage from knock-on recoil atoms. And finally, radiation shielding requirements can be determined.

A comprehensive analysis of intermediate-energy nuclear data needs for accelerator technologies is given by Koning in Ref. [24]. The Nuclear Energy Agency of the OECD has provided a leadership role in organizing and coordinating international intermediate-energy nuclear data activities for emerging accelerator technologies [25].

![Graph of FKK-GNASH calculations](image)

Fig. 9. FKK-GNASH calculations of the angle-integrated inclusive emission spectrum in the 160 MeV $^{90}$Zr$(p,xn)$ reaction, compared with measurements [22]. Contributions from different preequilibrium stages are indicated. Taken from Ref. [23].

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