Project Title:

Radiation Transport Modeling of Beam-Target Experiments for the AAA Project

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AAA Research Area: **Transmuter**

Requested First Year Funding: $ 109,979 (out years comparable)

Note: ANL employees do not require funding from UNLV to participate in this project.

Radiation Transport Modeling of Beam-Target Experiments for the AAA Project

Abstract

The AAA program will rely on the use of an accelerator-based transmuter[1] to expose spent nuclear fuel to high-energy neutrons. The neutron flux will be sufficient to activate or fission the long-lived isotopes of Tc, I, Pu, Am, Cm, and Np that present a significant safety hazard in commercial spent fuel. Transmuter fuel will be subcritical and a high-energy proton accelerator is needed to maintain the necessary neutron flux through the use of a neutron spallation target. The maximum neutron energy produced by spallation (~ 600 MeV) is significantly higher than that produced by a commercial light water reactor (~ 2 MeV). To design the nation's first transmuter, the neutronics code MCNPX will be used to model the distribution of neutron flux within the fuel blanket and to determine the neutron multiplication, k_{eff}. However, the cross section libraries and computational methods used by MCNPX at these neutron energies still have some uncertainty and will require validation.

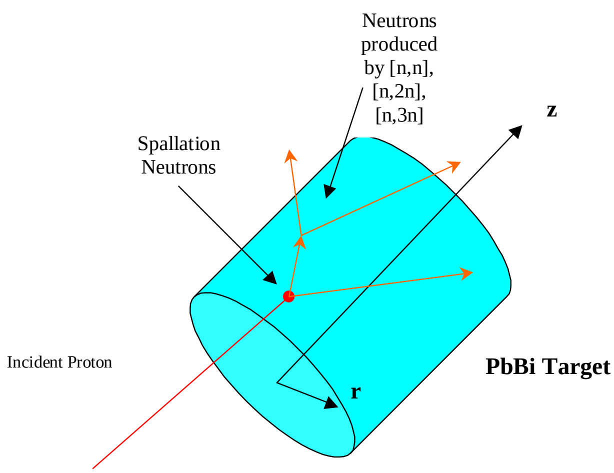

Figure 1. Leakage of High Energy Neutrons from a Spallation Target

To lessen the uncertainties in the MCNPX libraries, the Department of Energy, through its national laboratories, is in the process of conducting several experiments utilizing protons produced by the Los Alamos Neutron Science Center (LANSCE) accelerator at the Los Alamos National Laboratory. MCNPX simulations provide valuable information for the design of experiments in addition to their use in analysis of experimental to validate and improve the codes and databases. We propose a research project wherein UNLV students and faculty will contribute to these critical experiments by performing computational work using the latest versions of MCNPX and its associated data libraries. This research project will be conducted in close coordination with AAA leads and researchers in both experimental projects and code and database development.

Work Proposed for Academic Year 2001-2002, Goals, and Expected Results

High Energy Neutron Leakage from a Spallation Target

During the upcoming year, researchers at LANL are planning to assemble beam-target experiments to study the production of neutrons by high-energy protons. A team of researchers from LANL, Argonne National Laboratory (ANL), and Lawrence Livermore National Laboratory (LLNL) has developed concepts for seven irradiation experiments that may benefit AAA target/blanket development. In these experiments, protons from the LANSCE accelerator will impact a target, which will produce a pulse of neutrons. These neutrons will penetrate the target and surrounding experiments (materials exposure, etc.), and will then escape into surrounding space and shielding. The ability to calculate or predict the time-dependent characteristics of the resulting neutron population will be critical to the design of future facilities such as accelerator-driven experiments in the existing Zero Power Physics Reactor (ZPPR), a future Accelerator-Driven Test Facility (ADTF), and the AAA. Early studies in the proposed research program will provide information to these experimentalists to assist them in designing the experiments and the instrumentation (neutron and gamma-ray detectors) to support the integral experiment program. Experimental results will be used to validate computational codes and data libraries.

The experimental project that is currently underway at LANSCE is an experiment to measure the leakage of fast neutrons from lead-bismuth targets. As shown in Figure 1, at the high neutron energies (more than 600 MeV) expected in a transmuter, the mean free path for neutron absorption may extend beyond the dimensions of the spallation targets. Neutron leakage can lead to the production in steel structures supporting the target of hydrogen and helium which cause embrittlement. Scattering collisions ([n,n], [n,2n], [n,3n]) within the target also generate new neutrons, which leads to spatially-dependent heat generation.

In this series of experiments the flux of neutrons leaking radially from a Pb-Bi spallation target, their energy spectra, and their spatial distribution will be measured. Because the neutron mean free paths are on the order of 18 cm, targets with 10, 25, and 50 cm diameters will be used in the experiments to verify code predictions. The experiments will provide data on neutron leakage from the target and measured reaction rates. That experimental data will then be used to test the ability of MCNPX, a high-energy version of the Monte Carlo transport code, MCNP, developed at LANL for radiation transport simulation and analysis, to adequately predict neutron leakage at these high neutron energy levels.

These experiments are scheduled to begin in December, however, there is an opportunity for UNLV students to begin training in the use of the software in the fall, including modeling of the scheduled tests and prediction of results, then to visit LANL in December to participate in the experiments. The students may also provide MCNPX simulations to support additional LANSCE tests scheduled for April 2001. This will involve UNLV engineering students and a faculty mentor in practical MCNPX work early in the AAA experimental program.

The UNLV researchers will work with Dr. Ray Klann, an ANL researcher and co-PI on the LANSCE experiment. The work consists of modeling the components of the spallation target including the Pb-Bi eutectic and supporting structure. MCNPX is a Monte Carlo simulation code that predicts neutron flux and energy levels. The steps in the analysis include:

1. Define the geometry and composition of the target and surrounding structure.
2. Compute the neutron flux, $\phi(E_n, r, z)$, within the target, reaction rates within activation foils, and expected detector responses.
3. Compute the neutron current densities in the radial and axial directions (see Figure 1) as a function of energy and position.
4. Compare computed distributions from MCNPX with experimental data.
5. Assess the ability of ENDF/B neutron cross sections within MCNPX to predict the experimental data for high-energy neutrons.

The verification of neutron cross sections from 10 to 600 MeV is essential for ADTF design. These cross sections are used to assess whether the target and fuel blanket can be maintained critical (k_{eff}= 1) through the use of a proton beam. Recent data by Embid, Fernandez, and Gonzalez (1998)[2] at CIEMAT, for example, showed a discrepancy in neutron scattering cross sections between ENDF/B-6.4 and the Japanese library JENDL-3.2. They simulated a critical mixture of TRU actinides with a lead diffuser/cooler for transmutation work[3].

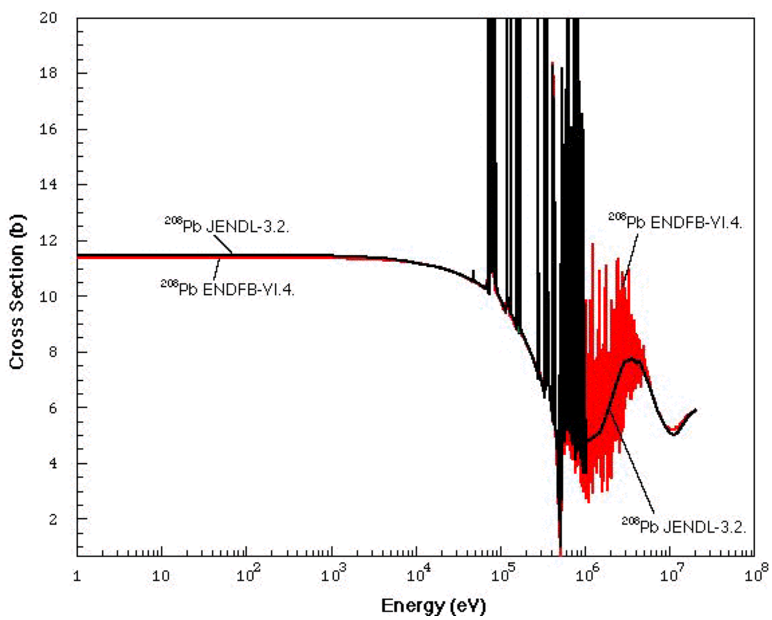

Figure 2. Differences in ENDF/B-6.4 and JENDL-3.2 Elastic Scattering Cross Sections for ^{208}Pb (http://fachp1.ciemat.es/texto.html)

As shown in Figure 2, deviations in the cross section libraries occurred above 1 MeV. *The discrepancy between the two libraries led to a deviation of 30% in the calculated values of k_{eff} for their ADS (accelerator driven system) using MCNP-4b*[4].

In addition to modeling of the spallation experiment, UNLV researchers would also be available to assist with the modeling of neutron detectors to assess their angular sensitivity.

Cross-Sections for the Activation of Sodium by Protons

Liquid sodium has been used as a coolant for fast reactors and its low Prandtl number and relatively high atomic number may make it ideal as a transmuter coolant. High-energy (~ 800 MeV) protons scattered by the spallation target will, however, produce activation products including tritium, Na-22, Be-7, and C-14. An experimental project is also scheduled for this year to study the production rate of these isotopes in sodium coolant. We propose to provide UNLV student support through MCNPX modeling to assist with this project.

Actinide Fission Cross-Section Measurement up to 100 MeV and Measurement of Multiplicity of Fission Neutrons in Actinides

These two AAA projects at LANSCE have been proposed for the next fiscal year. Actinide cross sections will be measured in Pu, Am, Np, and Cm for fission and for radiative capture. The second project involves measurement of the number of neutrons emitted per fission in actinides. Both experiments are necessary to verify MCNPX cross section libraries for high energy neutrons. LANSCE has instrumentation to complete neutron time-of-flight measurements to obtain the neutron spectrum, however, assistance will be required to post process the data and to complete unfolding of the neutron spectrum data. We propose to employ a UNLV graduate student and faculty member to work with the laboratory researchers to complete this work.

Laboratory and University Contacts

Dr. Ray Klann from the Argonne National Laboratory is co-principal investigator on several of the LANSCE experiments planned for this year. He is an expert in MCNPX usage and neutron detector design. Dr. Klann will be working with the UNLV students and with other researchers at LANL and ANL on the LANSCE beam line experiments.

Dr. Denis Beller from the Los Alamos National Laboratory will also work with UNLV students on this project. Dr. Beller is a nuclear engineer and he now serves as the liaison between the national laboratory efforts in AAA and the University of Nevada, Las Vegas. Dr. Beller is an experienced user of MCNP and he has provided modifications to nuclear codes that have been distributed nationwide by RSICC. He has worked closely with other researchers involved in the design of experiments at LANL and with radiation transport calculations.

The proposed project Principal Investigator is Dr. William Culbreth at the University of Nevada, Las Vegas in the Department of Mechanical Engineering. He has taught mechanical and nuclear engineering courses at UNLV for over 15 years. His research has included criticality calculations for the Yucca Mountain Project using KENO and SCALE 4.1, radiation transport studies for the Nevada Test Site, and simulations of the Oklo natural reactors.[5-10]

Research Objectives and Goals

For the first year of the proposed research, the goals are:

- Provide projections of expected time-dependent neutron flux, neutron absorption and fission rates, and reaction (fission and transmutation) rates inside the proposed LANSCE beam-target experiment, and neutron leakage spectra and rates from the experiment.
- Analyze results of the experiments.
- Validate computer codes for the simulation of accelerator-driven transmutation experiments and facilities.

The following objectives are identified to complete the goals:

- Acquire MCNPX for use on student workstations and provide for the adequate training of the student researchers.
- Work with Drs. Beller, Klann, Pitcher, and Wender along with other researchers at LANL and ANL to model the integral experiment at LANSCE.
- Conduct MCNPX simulations of the preliminary design of an integral experiment to estimate the neutron leakage from lead/bismuth targets of varying radii. Provide similar computational support for proton activation experiments in sodium coolant.

During Years 2 and 3, the goals will include analysis of the transient behavior of future experiments for control and safety, comparison of experimental data to MCNPX predictions for code validation, and MCNPX simulations of a proposed prototype transmuter. Neutron simulations will be proposed in support of the ZPPR (Zero Power Physics Reactor) experiments at INEEL to integrate UNLV students into this national user facility.

Technical Impact

Without the ability to predict the nuclear performance of subcritical assemblies driven by high-energy protons, the design of the ADTF and the future AAA systems cannot proceed. To gain a strong understanding of this coupled behavior, an integral experiment will be conducted at the LANL LANSCE proton beam facility. Beam-target experiments will be conducted to provide information for the design of these future facilities. The modeling of criticality, neutron absorption rates, and external gamma-ray and neutron flux will be very important in the design of these integral experiments. Through a comparison of predicted transmuter behavior to experimental data acquired from the experiment, MCNPX and its libraries can be validated and improved. This improved capability to predict nuclear performance is critical for the design of future experiments, and for the engineering design and licensing of the ADTF and AAA.

Research Approach

During the fall semester, students will be certified as part of the LANL MCNPX team and will then be trained in the use of MCNPX. During a visit with researchers at LANL, the students will be familiarized with the AAA project and the needs for radiation transport modeling in preparation for the LANSCE integral experiments. MCNPX modeling of the integral experiments will commence in the fall for the first graduate student working on the project with visits scheduled in December 2001 and April 2002 to support the neutron leakage experiments. A second graduate student will be sought to assist with the sodium activation experiments during the fall and to prepare for the "actinide cross-section" and "neutron multiplicity" studies early next year. Both students will work at UNLV and at LANL during the summer of 2002 to support the LANSCE beam line experiments. In collaboration with researchers at LANL, the computer simulations will be used in the design of the beam-target experiments including the placement of components and instrumentation.

Upon completion of the LANSCE integral experiments, the acquired neutron and gamma-ray spectra will be compared with the predicted results from MCNPX. Based on these comparisons, recommendations will be made regarding the use of MCNPX and its libraries for design of the ADTF and ATW. Analysis of the integral experiment data and simulations of ADTF would take place during Years 2 and 3 of the project.

Expected Technical Results

For the first year of the proposed work, the MCNPX computer code will be used to calculate the expected neutron flux, neutron and proton activation rates, and generated heat rates from LANSCE experiments. In collaboration with researchers at LANL and other institutions, these calculations will be used to support the design of experiments to be conduced at LANSCE and to optimize the design and placement of neutron activation foils and other instrumentation. Analysis of the data acquired during the experiments will be used to indicate areas of uncertainty in MCNPX and to design future transmuter experiments.

Capabilities at the University and Los Alamos

The LANSCE particle accelerator facility at LANL produces high-energy protons ideal for the development of a transmuter demonstration project. To carry out the proposed work, computer workstations located at UNLV will be utilized. If required, additional computing power will be obtained though the National Supercomputing Center for Energy and the Environment at UNLV.

Equipment Requested for AAA User Labs

Due to the computational requirements for the proposed work, two computer workstations are requested for the students working on the project. The computer workstations will be equipped with microprocessors with at least 1.4 GHz of speed and at least 1 gigabyte of random access memory. The MCNPX software and associated data libraries will be provided by the LANL MCNPX development team at no cost to the project.

Project Timeline

Timeline Narrative

Time is scheduled during the beginning of the project to train students in the use of MCNPX. The two students working on the project will also travel to LANL to visit with LANL researchers and to help familiarize themselves with the AAA project. Radiation transport modeling of the LANSCE experiments will commence by the third month of the project and continue through the year.

	Year 1											
Task	9/01	10/01	11/01	12/01	1/02	2/02	3/02	4/02	\5/02	6/02	7/02	8/02
Neutron Leakage Experiments												
MCNPX Training												
LANL/LANSCE Visits and Work												
Postanalysis of neutron data												
Sodium Activation Experiments												
MCNPX Training												
MCNPX (and other codes) modeling												
LANL/LANSCE Visit												
Analysis of Data												
Actinide Fission Measurements												
Neutron Multiplicity Measurements												
MCNPX Simulations												
LANSCE Site Visit												

Expected Technical Results

The results will include computational models of LANSCE beam-target experiments, recommendations for the design of the integral experiment to best model potential ADTF and AAA devices, and initial evaluation of the results of the integral experiment tests, if available during Year 1.

Milestones

The milestones include completion of student training in the use of MCNPX, completion of the literature review and familiarization, and commencement of radiation transport modeling of the LANSCE AAA experiments.

Deliverables

The products of the research will include quarterly reports that detail progress on the research, copies of publications, and summaries of collaboration with the national laboratories. A final annual report will be submitted by the 12^{th} month of the project. Student work, including copies of theses, dissertations, and senior design reports will also be included with quarterly progress reports.

Related Publications

1. U.S. Department of Energy, “A Roadmap for Developing Accelerator Transmutation of Waste (ATW) Technology,” DOE/RW-0519, October 1999.

2. M. Embid, R. Fernández, and E.M. González, “Sensitivity study for the K_{eff} of a lead based ADS on the cross sections evaluations: ENDFB-6.4 and JENDL-3.2,” CIEMAT (Madrid-Spain), CIEMAT REPORT 846 (1998).

3. C. Rubbia et al. *Conceptual Design of a Fast Neutron Operated High Power Energy Amplifier*. CERN/AT/95-44 (ET) (1995).

4. J. F. Briesmeister, Editor. MCNP™ — *A General Monte Carlo N-Particle Transport Code. Version 4B*. LA-12625 (1997).

5. Culbreth, W., and Viggato, J., “Determination of the Depth and Pressure within the Oklo Natural Reactors,” Proceedings of RPS2000, Spokane, Washington, September 2000.

6. Culbreth, W., and Steeps, L., “Nuclear Criticality at the Oklo Natural Reactors,” Proceedings of the International Conference on Nuclear Engineering, San Diego, CA, May, 1998.

7. Culbreth, W. G., and Zielinski, P. R., "Long-Term Effects of Poison and Fuel Matrix Corrosion on Criticality," Proceedings of the Fifth Annual International High-Level Radioactive Waste Management Conference, pp. 634-641, 1994.

8. Zielinski, P. R., and Culbreth, W. G., "Calculation of keff for Vitrified Plutonium Waste Packages," Proceedings of the Fifth Annual International High-Level Radioactive Waste Management Conference, pp. 679-683, 1994.

9. Culbreth, W. G., and Zielinski, P., "Analysis of the Criticality of a Spent Fuel Waste Package using Mathcad for Windows," Ninth ICMCM, Berkeley, CA, July 1993.

10. Culbreth, W. G., and Zielinski, P. R., "The Effect of Fuel Burnup and Dispersed Water Intrusion on the Criticality of Spent High-Level Nuclear Fuel in a Geologic Repository," Scientific Basis for Nuclear Waste Management XVII, Materials Research Society, vol 333, pp. 445-454, 1993.

July 12, 2001

Dr. Anthony Hechanova
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Las Vegas, NV 89154-4009

Dear Tony,

I have worked with Dr. Bill Culbreth on the development of the proposal "Radiation Transport Modeling of Beam-Target Experiments for the AAA Project." My main interest is to coordinate student and faculty activities at UNLV to support the small-scale irradiation experiments at the LANSCE facility. The tasks proposed identify activities that a student can perform and reflect the current focus and project planning for the experimental campaign. It is also worthy to note that the student will play an integral role in all aspects of a given experiment and will be relied upon for the successful execution and analysis of the experiments.

It is my hope that this will result in a great teaming relationship that will continue into the future. The AAA project will gain valuable and timely technical support, and at the same time Bill and his students will become involved in a challenging and important national project through their support of the initial small-scale experiments.

I strongly support the reference proposal and look forward to working with Bill and his students on this project. In addition, I would like to see more involvement in the AAA project on the part of UNLV faculty and students.

Thank you for your consideration in this matter and please feel free to contact me if you need additional information.

Sincerely,

Raymond T. Klann