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

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Proposal Narrative

Project Title:

**Project Continuation Proposal: Radiation Transport Modeling of Beam-Target Experiments for the AAA Project**

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AAA Research Area: Transmuter

Requested Year 2 Funds: $97,108
Abstract: The AAA program will rely on the use of an accelerator-based transmuter 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 radiological 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 (~ 800 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.

To remove the uncertainties in the MCNPX libraries, the Department of Energy, through its national laboratories, is in the process of conducting several experiments utilizing the proton and neutron beam lines at the LANSCE proton accelerator at the Los Alamos National Laboratory. MCNPX simulations of the experiments and post-processing of the acquired data are necessary and UNLV students and faculty on this project have been involved in this computational work.
Work Proposed for Academic Year 2002-2003, Goals and Expected Results:

High Energy Neutron Leakage from a Spallation Target

This project is currently underway at LANSCE and involves experiments to measure the leakage of fast neutrons from lead-bismuth targets. As shown in figure 1, at the high neutron energies (800 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 of hydrogen and helium in steel structures supporting the target causing embrittlement. Scattering collisions ([n,n], [n,2n], [n,3n]) within the target also generate new neutrons leading to spatially-dependent heat generation.

The experiments will test the ability of MCNPX to adequately predict neutron leakage at these high neutron energy levels. The flux of neutrons leaking radially from a Pb-Bi spallation target, their energy spectra, and their spatial distribution will be measured in a series of experiments. Since the neutron mean free paths are on the order of 18 cm, targets with 10, 20, and 40 cm diameters will be used in the experiments to verify code predictions.

Experiments began in December, 2001 at LANSCE and additional targets are scheduled for July 2002 and possibly December 2002. UNLV students have been conducting MCNPX simulations of the 12/01 tests to verify neutron flux measurements and the energy spectra measured by two time-of-flight detectors.

The UNLV researchers have worked with Dr. Ray Klann, an ANL researcher and co-PI on this LANSCE experiment, Dr. Denis Beller from LANL and head of the nationwide university programs in AAA, Dr. Eric Pitcher from LANL, and Dr. Michael James from LANL. Several UNLV students have worked on the project.

- Jason Viggato, a doctoral student in mechanical engineering, is scheduled to finish his degree in August 2002. He worked on the project for two semesters before accepting a job at Bechtel SAIC in April 2002.
- Daniel Lowe, an undergraduate mechanical engineering student, is currently a junior. He has become an invaluable resource with an expertise in MCNPX. He
will spend much of the summer at LANSCE to document the neutron leakage experiments and to conduct MCNPX simulations. He is scheduled to graduate in May, 2004.

- Suresh Sadenini, a masters student in mechanical engineering, is scheduled to graduate in December 2002. He has worked on the project since December 2001 and has assisted in MCNPX simulations of the LANSCE neutron leakage tests. He will be working on his thesis project this summer at the Idaho Accelerator Center with support from Dr. Frank Harmon.

- Ashraf Kaboud, a master student in mechanical engineering, is beginning work on the project as of May, 2002. He is scheduled to graduate in May 2003 and will assist in MCNPX modeling.

The work on the project has consisted 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 have included:

1. Define the geometry and composition of the target and surrounding structure. The target composition, for example, is made up of various natural isotopes that must be incorporated into the models.
2. Compute the neutron flux, \( \phi(E_n, r, z) \), within the target and at the target surface as a function of neutron energy and spatial position.
3. Compute the neutron energy spectra from at the location of time-of-flight detectors used in the experiments.
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 800 MeV is essential for ATDF design. These cross sections are used to assess whether the target and fuel blanket can be maintained critical (\( k_{\text{eff}} = 1 \)) 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

![](http://fachp1.ciemat.es/texto.html)
As shown in figure 3, 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 $k_{\text{eff}}$ for their ADS (accelerator driven system) using MCNP-4b\(^5\).

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.

**Actinide Fission Cross-Section Measurement up to 100 MeV**

**Measurement of Multiplicity of Fission Neutrons in Actinides**

These two AAA projects at LANSCE have been proposed for the future, contingent upon funding. 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. If these tests move forward during the upcoming year, we propose to employ a UNLV graduate student and faculty member to work with the laboratory researchers to conduct MCNPX simulations to help with this work.

**Funding Profile:**

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**Background and Rationale:**

The vision of ATW (Accelerator Transmutation of Waste) involves the remediation of high-level nuclear waste through the transmutation of actinides and radioisotopes with long half-lives into a product stream with much shorter half-lives. By using a proton accelerator, a subcritical blanket of spent fuel can sustain a stable flux of fast neutrons to transmute the waste. The safe operation of such a device is ensured since a subcritical assembly is incapable of sustaining a chain reaction without the spallation neutrons created by a proton accelerator.

Radiation transport studies are needed of the proposed ATW facility and for analyzing potential advantages to using the LANSCE proton accelerator at Los Alamos National Laboratory (LANL) in combination with integral beam-target experiments in preparation for integral beam-target-multiplier experiments at other facilities. The proposed studies will be accomplished through the use of MCNPX, a high-energy version of the Monte Carlo transport code, MCNP, developed at LANL for radiation transport simulation and analysis.
The Integral Beam-Target Experiment

During the upcoming year, experimentalists at LANL are planning to continue 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) have developed concepts for seven irradiation experiments that may benefit AAA target/blanket development. These experiments are contingent upon federal funding and a single neutron leakage test has been conducted to date in December, 2001.

In the planned 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), the future ADTF (Accelerator-Driven Transmutation Facility), and the ATW. 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 the MCNPX code and its data libraries.

Figure 4 ProEngineer CAD Image of the Pb/Bi Neutron Leakage Target
(Yellow line is proton beam path, red components are aluminum, blue components are steel, and yellow circles are detector positions used in MCNPX)

Figure 5 Neutron Leakage Tests Results Are Affected by Other Objects In Proximity to the Target
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 has worked with the UNLV students on the project and with other researchers at LANL and ANL on the LANSCE beam line experiments. Dr. Eric Pitcher at the Los Alamos National Laboratory has also worked with the students on the project and assisted in running the MCNPX code.

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 project Principal Investigator has been 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

Work Completed During the First Year of the Project

UNLV faculty and students have accomplished a number of tasks during the first year of the project. The project began in late August, 2001 and work will continue through this summer on the first year of the project. During the summer, Daniel Lowe (student researcher) will spend 6 weeks at LANSCE and Suresh Sadenini (graduate student researcher) will spend 3 months at the Idaho Accelerator Center at their expense.

Figure 6  Neutron Flux Through Pb/Bi Target Surface
(Z = distance (cm) from proton beam impact point on front of target, T = angle (degrees) where 180 corresponds to bottom of target)
During the fall of 2001, several students were trained in the use of Monte Carlo codes for radiation transport analyses. The ORNL nuclear criticality code, KENO-V, was initially used to train the students in the use of ENDF/B neutron cross section libraries, geometry definition, and in the definition of tables defining common engineering materials. This code was used awaiting the acquisition of high speed computers and the MCNPX radiation transport code.

In October, UNLV became a member of the beta test team for MCNPX headed by Dr. Laurie Waters at LANL.

Two high-speed (1.8 GHz) computer workstations were purchased for student use on the project in November.

In November 2001, Dr. Culbreth and the students attended the Student Mini-Conference at the annual American Nuclear Society meeting in Reno, Nevada. Three students presented papers on their work at UNLV on transmutation (D.Lowe, L. Bakker, and J. Viggato). The talks were also presented as posters at the meeting. J. Viggato won an award for the best presentation within his section.

A networked 800 MHz computer was acquired and equipped with the LINUX operating system for student and faculty use on the project. A beta version of MCNPX was installed on the computer.

Figure 7  MCNPX Simulations of the Measured TOF (Time-of-Flight) Detector Neutron Energy Spectra
In December, 2001, Dr. Culbreth and students Daniel Lowe, Elizabeth Bakker, and Jason Viggato visited with Dr. Ray Klann at the Argonne National Laboratory in Chicago. Dr. Klann provided the UNLV team with sample MCNPX input files for the simulation of the neutron leakage experiments.

In December, 2001, Suresh Sadenini, a UNLV mechanical engineering graduate student, joined the research team. Through Dr. Beller at UNLV, we began communicating with Dr. Frank Harmon, Director of the Idaho Accelerator Center. The IAC is one of a handful of university-affiliated laboratories cooperating in the nationwide studies on the accelerator-based transmutation of nuclear waste. Dr. Harmon invited Suresh and Dr. Culbreth to visit the IAC and our visit in December resulted in an offer for Suresh to work at the IAC during the summer of 2002 on an experiment that will result in his thesis project. Dr. Harmon will use a high-voltage electron source to impact a solid lead target to produce neutrons. This experiment will test the feasibility of using an electron beam to subsequently produce neutrons that can be used in a transmuter. Suresh’s work will involve MCNPX simulations of the experiment to compare with the measured neutron flux and validate the use of the code for transmuter designs based on particle beam accelerators. Suresh will complete his masters degree in December, 2002.

In January, 2002, Dr. Waters and her MCNPX team taught an introductory MCNPX class at UNLV. Dr. Culbreth and four students completed the course and acquired a working copy of MCNPX for the PC-based student workstations. Student participants included S. Sadenini, J. Viggato, D. Lowe, and L. Bakker.

Dr. Klann visited with the students and Dr. Culbreth in February and in April 2002 to discuss the research. These visits included discussions of the preliminary LANSCE neutron leakage test results contained in a report prepared by Dr. Klann and others based on the December tests.

A sample plot of neutron flux prepared by D. Lowe through the target surface is shown in Figure 6. The contour plot shows the change in flux through the surface as a function of axial distance, Z, from the proton beam impact point and as a function of angle, T. The angle is 180° at the bottom of the target. A steel table located below the target is responsible for reflecting neutrons back into the target contributing to the flux. This created a difference in flux of about 2% from the bottom to the top of the cylindrical Pb/Bi target.

Time-of-flight detectors are located roughly 50 m from the target and their measurements are influenced by other objects in and around the “Blue Room”. Figure 7 shows the results of MCNPX runs on the neutron energy spectra expected at the two TOF detectors used in the December 2001 neutron leakage tests. The results are in good agreement with the measured values (not yet published) and will be improved by completing the full geometry of the room into the MCNPX model.
• Based on discussions with Dr. Klann, D. Lowe began preparing a CAD drawing of the “Blue Room” at LANSCE. Figure 4 and 5 show 3-D images of the target and the target table. A large steel sphere located in the room contributed to an anisotropy of about 1% in the neutron flux through the surface of the target.

• In April, 2002, our doctoral student, Jason Viggato, accepted a job at Bechtel SAIC working on the Yucca Mountain project. He received this job based on his experience with MCNPX, SCALE 4.1, and heat transfer codes. He is expected to complete his doctorate this summer.

• In May, 2002, Dr. Eric Pitcher (LANL) assisted several AAA projects on campus in the use of MCNPX. Dr. Pitcher also discussed foil activation studies with us based on the December 2001 LANSCE neutron leakage tests.

• Through conversations with R. Klann and M. James, Daniel Lowe will spend 6 weeks at LANSCE to complete his CAD images of the Blue Room, to conduct MCNPX simulations and to assist with the July neutron spallation tests. His work will also help in the preparation of a benchmark program for these tests.

Proposed Work in Year 2 of the Project

Dr. Klann provided us with a list of simulations to conduct that will be completed during the summer for the December 2001 neutron leakage tests. Similar simulations will be conducted during Year 2 for the July and December 2002 tests.

1. Model targets of varying diameter in air, in a vacuum, and in the presence of humid air.
2. Model various proton beam profiles.
3. Model the effects of off-axis proton beam impingement on the target.
4. Model the asymmetry introduced by the steel table below the target.
5. Model the effect of varying ratios of Pb to Bi and the effect of impurities.
6. Model the system including other structures within the test room.

Dr. Eric Pitcher asked that we compute the activation induced by neutrons passing through the sets of foils attached to the spallation target. Activation is a function of the incident neutron energy and the MCNPX simulations will include this effect. We propose to conduct this work during the summer and during Year 2 for the next series of neutron leakage tests.

We will proceed during the summer and during Year 2 with the development of a benchmark program for the neutron leakage tests and for other tests related to transmuter development. This program will parallel the international benchmark experiments and modeling conducted by the OECD Nuclear Energy Agency and cooperating laboratories. A comprehensive three-dimensional CAD image of the LANSCE experiments will be prepared using ProEngineer during the summer and fall to help
benchmark the experiments and to provide accurate geometric data for MCNPX modeling.

Other research work to be completed during Year 2 includes MCNPX simulations of spallation targets in preparation for the 12/02 neutron leakage tests and we are very interested in assisting with the neutron multiplicity and actinide fission cross-section experiments. There has been some planning to conduct neutron multiplication tests at the IAC using an electron accelerator and a subcritical blanket. One of our students will be spending the summer at IAC and we would like to assist with modeling and data reduction, if the tests are conducted in Year 2 of this project.

**Research Objectives and Goals:**

During the first year of the research project, the goals were to:

- 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.

As indicated above, computer workstations were purchased and the MCNPX software installed. Students and faculty were trained in the use of MCNPX. Dr. Klann provided sample input and output files and assisted the UNLV team in the simulation of the neutron leakage experiments.

Much of the work scheduled for year 1 of the project will be conducted during the months of June through August of this year. Daniel Lowe is traveling to LANSCE for a six week period starting on June 15 to document components in the Blue Room in preparation for the next neutron leakage experiment to be conducted in early July. Suresh Sadineni will be working at the Idaho Accelerator Center for three months to help with the experiments on the production of neutrons with an electron accelerator. Dr. Culbreth and Ashraf Kaboud will remain at UNLV and complete the studies.
recommended by Dr. Klann to complete work on the experiments of December, 2001 at LANSCE.

During the second year of the project, the goals include:

- Continue analyses of the neutron leakage tests completed in July 2002 and to be conducted on LANSCE in December, 2002.
- Prepare simulations of the December 2002 tests to provide input on the test design.
- Complete work started in the first year on a benchmark program for the validation of MCNPX for transmutation studies. This program will be designed along the lines of the international nuclear criticality benchmark series.

**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 ATW 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 for use in the design of experiments, the ADTF, and ATW.

**Research Approach:**

The research approach involves the use of the MCNPX computer code for the simulation of criticality and other nuclear properties of proposed LANSCE experiments to be conducted at LANL. ProEngineer will also be used to provide three-dimensional CAD images of the benchmark tests.

**Expected Technical Results:**

For the first year of the proposed work, the MCNPX computer code will be used to provide estimates of 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 estimates will be used to support the experiments to be conducted 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 through the National Supercomputing Center for Energy and the Environment at UNLV.

Equipment Available in the UNLV/AAA User Labs:

Due to the computational requirements for the proposed work, two computer workstations were purchased during year 1 of the project. Both computers are used by the students on the project and have a processor speed of 1.8 GHz. The machines have the most recent version of MCNPX installed with both ENDF/B-6 and LA-150 cross section libraries. One machine has a copy of TECPLOT installed. This software is used to generate color contour plots as shown in Figure 6. One machine currently has a copy of ProEngineer installed. Daniel Lowe used ProEngineer to create three-dimensional CAD drawings of the Blue Room at LANSCE as shown in Figures 4 and 5.

Project Timeline:

Timeline Narrative:

Year 1 of this project began in late August at the beginning of the academic year at UNLV. Students began the year by learning how to use radiation transport codes. During the winter break, students received formal training in MCNPX and visited the Argonne National Laboratory to discuss the research.

During the summer months of 2002, two of the students will be at LANSCE and the IAC (Idaho Accelerator Center) to conduct work. The student working at IAC is also assisting in the LANSCE experiment simulations using MCNPX. He has been supported for 10 hours per week during the spring semester from the AAA project and he will be supported by the IAC during the summer. The timeline for the end of Year 1 and through Year 2 is shown below.

Much of the work scheduled for Year 2 of the project will include benchmarking of the experiments conducted at LANSCE, simulation of proposed LANSCE tests, and comparison of experimental results to MCNPX models.

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 ATW devices, and evaluation of the results of the integral experiment tests.
Milestones:

The milestones include completion of MCNPX simulations and the preparation of benchmark tests as shown in Table 1.

Table 1 Timeline for the End of Year 1 and Through Year 2 of the Project

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<td>3. Benchmarking of neutron leakage tests</td>
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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 12th month of the project. Student work, including copies of theses, dissertations, and senior design reports will also be included with quarterly progress reports.


Literature Cited:


July 12, 2001

Dr. Anthony Hechanova
Harry Reid Center
University of Nevada - Las Vegas
4505 Maryland Parkway - Box 454009
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