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Development Of A Novel Genetic Algorithm-based Optimization Method For Design Of Nuclear Criticality Experiments

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A new evaluation of isotopic molybdenum total neutron cross section data based on measurements performed at Rensselaer Polytechnic Institute prompted researchers at Rensselaer and Los Alamos National Laboratory (LANL) to design a nuclear criticality experiment for the validation of the data. A novel approach of criticality experiment design employing a genetic algorithm-based optimization technique was developed. The method produced a critical experiment with a cross section sensitivity that exceeded target specifications by an order of magnitude.

I. MOTIVATION

Nuclear data is the foundation of nuclear engineering calculations and is utilized in all nuclear engineering disciplines, including reactor modeling, criticality safety, health physics, and radiation detection. [1] Because nuclear data is the basis of accurate modeling and simulations and due to the inherent safety risks associated with nuclear systems, it is vital that the nuclear data is as accurate as possible. The fundamental parameters of nuclear data, known as cross sections, describe the probability of a given type of interaction and are material, particle, and energy dependent and are subject to rigorous validation and verification.

Historically, a popular method of cross section validation has been the design and use of critical experiments that are sensitive to the specific cross sections to be validated. [2,3] These critical assemblies are designed such that their neutron multiplication factor k_{eff} is highly sensitive to the cross sections of interest, meaning that a small inaccuracy in the cross section value will produce a large change in k_{eff}. Experimental measurements of k_{eff} are compared to simulation results using different nuclear data libraries in order to benchmark the data.

Intermediate energy measurements of isotopic molybdenum total neutron cross sections from 1 keV to 620 keV at Rensselaer created a need for a system to validate the new data. [4] Intermediate energy data is especially important to the modeling of fast and intermediate reactor systems, criticality safety and prediction for non-thermal spectra, and fission neutron slowing-down. Because of the complexity of critical assemblies, the design of a highly-sensitive system can be extremely tedious. As a result, a new method applying genetic algorithm optimization to experiment design has been developed and utilized to design a system highly sensitive to unresolved resonance region (URR) molybdenum capture and elastic scattering cross sections from 1 to 100 keV.

II. SYSTEM GEOMETRY

While criticality experiments can be designed in a wide range of geometries, the project was initiated with the intention of utilizing LANL'S Comet vertical assembly machine, shown supporting the Zeus critical experiment in Figure 1. [5]

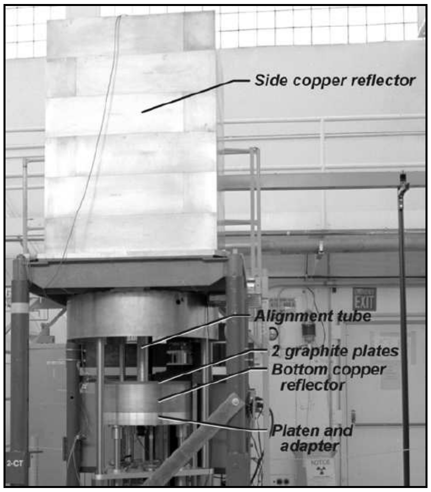

Figure 1: The Zeus critical experiment atop the Comet vertical assembly machine.

An axial cross section of an example system is shown in Figure 2.

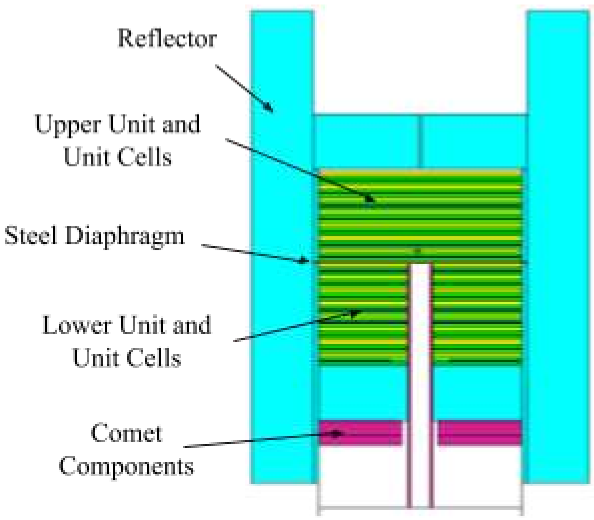

Figure 2: Vertical cross section of a critical assembly using Comet.

Comet constrains the geometry of the system to be of a cylindrical, stacked design surrounded by a large reflector, as shown in Figure 2. A steel diaphragm in the center of the reflector divides the system into an upper, stationary unit and a lower, mobile unit. These assembly units consist of stacks of unit cells, or smaller stacks of plates of Highly-enriched uranium (HEU) fuel, moderator material, and the material of interest. The unit cells have a repetitive structure such that they possess a well-defined reactivity worth for an approach to critical process as the lower unit is raised into the system by Comet.

The set of Zeus experiments were used to define the components of the optimization problem for the new experiment.

III. OPTIMIZATION METHOD

The optimization problem was rigorously defined with the system sensitivity chosen as the optimization parameter. The sensitivity s to a particular cross section σ is expressed mathematically as the ratio of relative changes in the multiplication factor and the cross section, as shown in Equation 1.

$$s(E) = \frac{\Delta k_{eff}/k_{eff}}{\Delta\sigma(E)/\sigma(E)} \quad (1)$$

Because the cross sections and subsequently the sensitivity are both reaction-type and energy dependent, the maximum magnitude of the energy-dependent capture sensitivity profile in the intermediate energy region was chosen to be the optimization parameter. Design variables for the optimization were the moderator plate thickness, molybdenum plate thickness, and number of unit cells in the upper and lower units. A schematic of a unit cell is shown in Figure 3.

Figure 3: Schematic of a unit cell.

Teflon, beryllium, Lucite, and graphite were explored as candidate moderator materials. Operationally, the system was constrained to reach criticality within a $0.80 excess reactivity margin. The main geometric constraints imposed on the system were maximum weights of the upper and lower assembly units of 20,000 and 2,000 pounds, respectively, and additionally the system was required to fit within the surrounding reflector. The system was modeled mathematically with the Monte-Carlo transport code MCNP® 6.1.1-Beta [6].

This optimization problem was classified as a gradient-free, mixed integer, multi variable optimization problem. A common optimization technique applied to this classification of problems is a genetic algorithm, as genetic algorithms are gradient free methods that are flexible to accommodate multiple continuous and discrete design variables. [7]

Genetic algorithm optimization is based on the theory of evolution. Initially, the algorithm randomly generates a population of *n* members where each member is a vector $\vec{x}$ of design variables and each design variable is within user-set bounds. The algorithm performs function evaluations on each member using the problem's mathematical model and characterizes each member by its fitness, or how well the optimization parameter is maximized or minimized. The algorithm mates the members in the population based on fitness via crossover and mutation algorithms, producing child members whose design variable values are an aggregate of that of their parents. Function evaluations are performed on the child members, and by comparing fitness, the algorithm selects a certain number of members out of the whole population to move to the next generation. This process is repeated until the optimal population member does not change over a user-defined number of generations.

Genetic algorithms are advantageous because of their flexibility to handle a wide range of problem types and can sample a wide range of candidate design space. Disadvantages of genetic algorithms are increased computational time due to the need for many function evaluations and the fact that they are an unconstrained method of optimization, meaning that an external method must be applied to enforce the constraints. A common method of handling constraints is the quadratic penalty method for inequality constraints in minimization algorithms defined in Eq. 2, where $\Phi(\vec{x})$ is the penalized objective function value, $J(\vec{x})$ is the raw objective function value, μ is a user-defined penalty parameter, and is the i^{th} of m inequality constraints.

$$\Phi(\vec{x}) = J(\vec{x}) + \frac{\mu}{2} \sum_{i=1}^{n} min(\hat{c}_i, 0)^2 \qquad (2)$$

Inequality constraints are formulated such that they evaluate positive if satisfied and negative if violated. Equation 2 shows that if a constraint is satisfied and is positive, no penalty is applied, whereas if a constraint is violated and evaluates negative, a penalty is applied. For minimization algorithms, this penalty is adding to the value to be minimized, thus decreasing its fitness. In this application to maximize the sensitivity, the same method is applied except the optimization parameter is negated. This method is advantageous because, in the event of a dissatisfied constraint, the magnitude of the penalty contains information as to the magnitude of the constraint violation. As a result, the algorithm can utilize this information to converge toward an optimum.

A code suite was developed to facilitate the optimization of the criticality experiment which employs the discussed approach. The results of the optimization are discussed in Section IV.

IV. RESULTS

The optimization method produced four assembly systems, one for each moderator material under consideration. The designs were compared by performance based on technical specifications. Table I shows the performance specifications of each optimized design, specifically the excess reactivity ρ_{ex} in units of dollars, upper unit weight W_U and lower unit weight W_L in units of pounds, and maximum total sensitivity magnitude S_{max}.

Table I: Optimized system performance specifications for each candidate moderator material.

	Teflon	**Graphite**	**Beryllium**	**Lucite**
ρ_{ex}	0.244	0.164	0.536	0.214
W_U	17236	17221	16577	16126
W_L	1218	1270	1043	834
S_{max}	0.0170	0.0139	0.0132	0.0068

Table I shows that for each candidate moderator material, the genetic algorithm produced a system that was critical within an $0.80 excess reactivity margin and met Comet imposed weight constraints. Although it was imperative that each design met these constraints, a choice between the moderator materials was based solely on the maximum intermediate energy total sensitivity magnitude. The Teflon-moderated system possessed the largest maximum sensitivity of 0.0170 and was subsequently pursued for the final design. Figure 4 shows the sensitivity energy profile for both capture and elastic scattering reactions in isotopic molybdenum for the Teflon-moderated system.

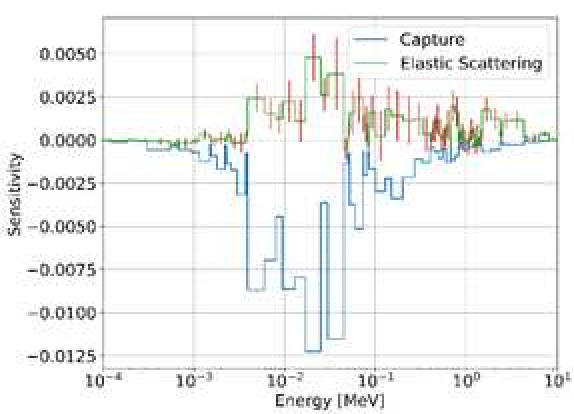

Figure 4: Sensitivity profile of optimized Teflon-moderated design.

Figure 4 shows that, for the Teflon-moderated system, the capture sensitivity typically has a larger magnitude than the elastic scattering sensitivity, due to the larger cross section magnitude in molybdenum for capture as compared to elastic scattering. Additionally, the elastic scattering sensitivity is positive over the energy range, while the capture sensitivity is negative. Positive or negative sensitivities indicate an increase or decrease in k_{eff}, respectively, due to inaccuracy in the cross section.

The maximum total sensitivity magnitude of 0.0170 for this system exceeds the target specification of 0.001 by more than a factor of 10. The sensitivity profile of the final design peaks at approximately 20 keV and possesses the highest sensitivities for energies between 5 and 80 keV, making this system sensitive across nearly the entire URR range from 1 to 100 keV.

V. CONCLUSIONS

The use of a genetic algorithm for criticality experiment design was shown to produce a system that met all technical specifications and constraints in addition to exceeding the target sensitivity by more than a factor of 10. Additionally, the sensitivity energy distribution possessed high sensitivity across the experiment region of interest, 1 to 100 keV. Traditional design of critical experiments can be tedious and time-consuming, whereas this method requires very little user configuration time and can produce an optimized design autonomously.

Future work in developing this methodology includes researching the scaling potential of this method for use with High-performance computing clusters (HPCs). Due to the significant computational resources required in genetic algorithm optimization, HPCs would be a solution to reducing computational time. Additionally, work on tailoring the genetic algorithm to provide the most robust results for a criticality experiment - specific problem is of interest.

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