A NOVEL MULTILEVEL SAFETY-FACTOR CENTERED FRAMEWORK FOR OPTIMIZED UTILIZATION OF RESEARCH REACTORS

by

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ABSTRACT

Nuclear research reactors are found throughout the world and have been crucial in the advancement of scientific and engineering discoveries but the majority are approaching operational ages that require a renewed focus on safely maintaining and optimizing their use. A novel multilevel safety-factors-centered framework for the optimization and utilization of aging research reactors has been developed that can be implemented at any research reactor facility. The framework consists of an optimization tool for neutron activation analysis (NAA) and irradiation experiments, an optimization system, DACOS, for optimizing reactor operation parameters, and the overall Engineering Safety Culture ideology.

The selection of NAA experimental parameters for irradiation in research reactors is essential in lowering the radiation dose to personnel while also minimizing the generation of excessive radioactive products. This comes in competition with assuring that enough activity of an examined sample is produced in order to be able to measure targeted trace nuclei. This is accomplished by coupling a NAA precalculator tool, PyNIC, with the optimization tool, DAKOTA, creating the PyNIC-DAKOTA tool system. This PyNIC–DAKOTA tool system is used to determine the optimal parameters for NAA. The PyNIC–DAKOTA tool system is benchmarked with several examples using the University of Utah TRIGA Reactor (UUTR). The PyNIC–DAKOTA tool system shows expected agreement with the actual NAA experiments.

DACOS is a newly developed computational optimization system that merges well-known neutron transport code AGENT and well-known optimization tool DAKOTA. The DACOS can be applied to any reactor configuration for the purpose of optimizing its operation parameters such as but not limited to determining the optimal fuel composition and spatial distribution, amount and position of reflectors and neutron absorbing materials to achieve a specified neutron flux at a given location in the reactor or reactor power level. DACOS demonstrations of application are given for modeling of the UUTR.

All of the research reactor optimizations and improvements are housed under the umbrella of a newly formed concept of Engineering Safety Culture and the workflow process that it encompasses. This new ideology is presented with illustrative examples of its implementation and resulting benefits.

This work is dedicated to my wife, Melissa, for her unwavering support and perseverance throughout this journey. She has been my rock, support and voice of encouragement that has allowed me to complete this work. I will always look up to and admire her for all the selfless work and effort she puts into supporting me and our family.

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CHAPTER 1

INTRODUCTION

Nuclear research reactors built in over 60 countries (Figure 1.1) have been operating for approximately 60 years in playing an imperative role in scientific and engineering advancements of human lives and technology. There are a wide array of designs with different operating modes such as steady state or pulsed. The most common design type is where the reactor core is a heterogeneous assembly of fuel elements submerged into a large pool of water that serves as a moderator and radiation shield.

Training, Research, Isotopes, General Atomics (TRIGA) reactors were developed in the late 1950s and constructed through the 1980s in 23 diverse countries, and many of them have continued to operate successfully for approximately 60 years [1]. TRIGA reactors have been utilized and built due to the following advantages: low capital cost, low operating costs, low fuel burnup, simple to operate, versatile, inherently safe, and less restrictive containment and siting requirements.

Many research reactors were built in the 1960s and 1970s with the peak of 373 reactors in 1975, compared with the current number of 245 as of 2016. Approximately 70% of operational research reactors are over 30 years old and more than 40% are over 40 years old [2].

Research reactors are utilized throughout the world for a variety of purposes.

These reactors are utilized for training, education, research, development, and industrial applications. Research reactors contribute to almost every field of science including physics, chemistry, geology, biology, archeology, medicine, and environmental sciences. Listed are a variety of activities and experiments that research reactors are performing:

- Neutron Activation Analysis (NAA) – a nondestructive, precise and accurate analytical technique capable of determining small quantities of up to 30 elements in almost all types of sample matrices [3].
- Production of short lived radioisotopes – short lived radionuclides are commonly used for tracer research at universities and hospitals, demonstration experiments, and teaching [4].
- Nondestructive testing by neutrons – a diagnostic technique that utilizes the reactor as a source of collimated neutrons and improves the knowledge of materials and structures and defects in various objects [5].
- Boron Neutron Capture Therapy (BNCT) – treatment for malignant melanomas and brain tumors by injecting the tumor with a borated compound and then irradiating with thermal neutrons [6].
- Training students and researchers – a research reactor can supplement theoretical courses with practical exercises for reactor theory and physics.
- Gemstone Irradiation – the color of crystals and semiprecious stones can be enhanced by epithermal and fast neutron irradiation [7].

Most operating research reactors are facing challenges due to the negative impacts of component and system aging. An example of how the issue can cause larger ramifications is when a serious medical isotope supply crisis was reached in mid-2010 due to several major producing reactors undergoing prolonged shutdowns due to extensive necessary repairs and overhauls [8]. There is no existing method or framework that provides aging parameter studies or evaluates the uncertainties for aging research reactors and their components. Very strict government-agency driven inspections of the research reactors are heavily based on inspecting the operational protocols but hardly address the framework for a prevention of the operational uncertainties due to the reactors' components aging. Little work or effort has been put forward into optimizing the operation and use of research reactors in getting the most out of the aging research reactor fleet.

1.1 Objectives

A novel multilevel safety-factors-centered framework is developed that can be applied to any of the existing research reactors; the framework provides a know-how assessment of how to approach and address any reactor operational or maintenance concern or problem and, in turn, optimize the use of the reactor as seen in Figure 1.2. The specific objectives of this work are the following:

1. *Design of Experiments:* Enhancing research reactor and radiological safety through the development of an optimization tool neutron activation analysis (NAA) and other irradiation experiments in research reactors [9], [10].
2. *DACOS (DAKOTA-AGENT Computational Optimization System) Optimization of Reactor Operation Parameters:* Advancing reactor operations and support the design of experiments by development of a robust and flexible neutronics computational optimization system applicable to reactor redesign or design,

modification and refueling [11], [12].

3. *Engineering Safety Culture Workflow:* Develop Engineering Safety Culture enhancement practices and workflow process to augment and improve research reactor facility conditions, operations, experiments, material accountability, waste storage, training, education, and opportunity for innovations [13]-[18].

1.2 Organization of dissertation

The development and theory behind the NAA optimization tool is presented in Chapter 2 along with benchmark tests of the newly developed system. Chapter 2 content is under review in the European Physical Journal – Nuclear Sciences and Technologies (EPJ N) [10]. Chapter 3 elaborates the design and development of the neutronic computational optimization system DACOS and also provides various benchmarks associated with the DACOS. Chapter 3 was published in the Annals of Nuclear Energy journal [12]. The Engineering Safety Culture theory, implementation and workflow process is given in Chapter 4. Chapter 5 provides the conclusion and describes future work that is planned for improving Engineering Safety Culture best practices.

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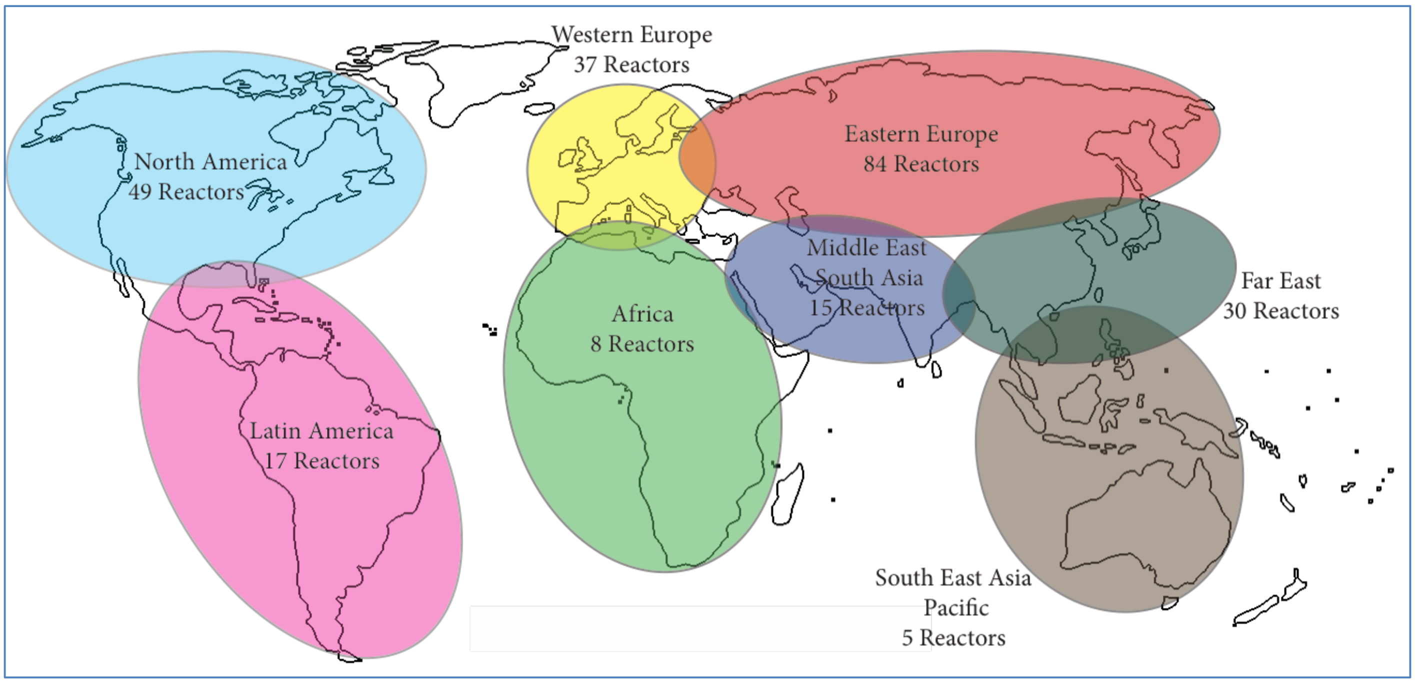

Figure 1.1: Word map of operating test and research reactors

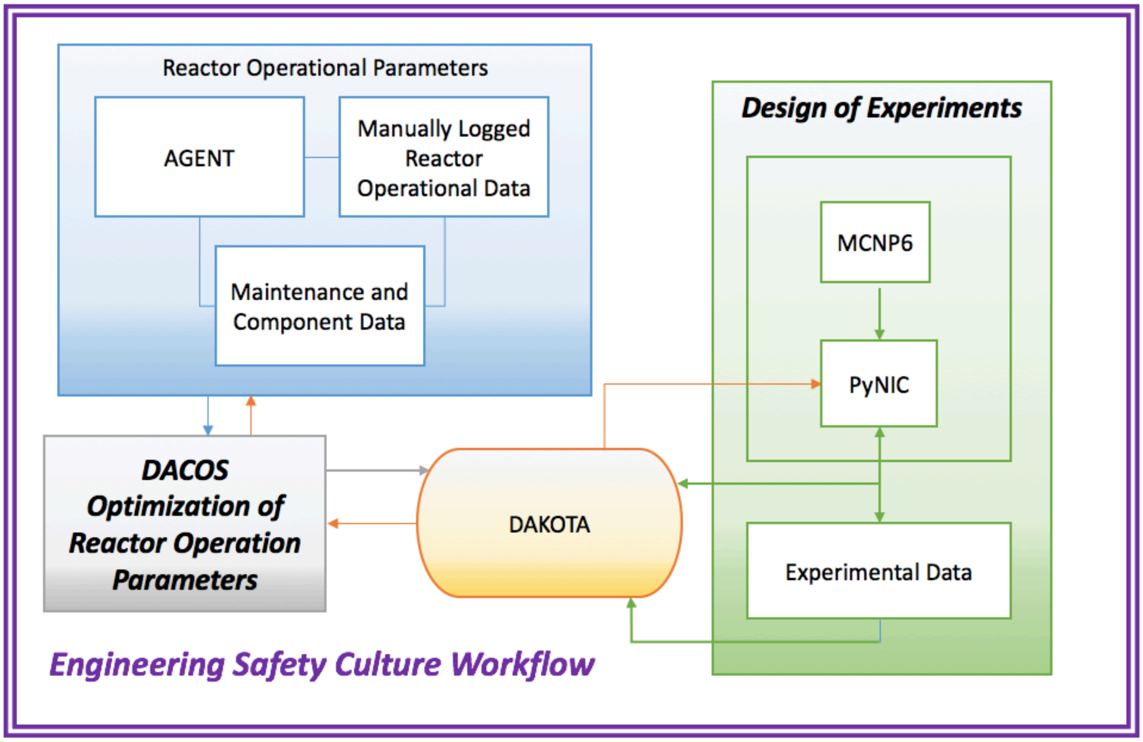

Figure 1.2: A novel multilevel safety-factor-centered framework for optimized utilization of research reactors; comprised of design of experiments (Chapter 2), DACOS (DAKOTA-AGENT computational optimization system) optimization of reactor operation parameters (Chapter 3), and Engineering Safety Culture workflow (Chapter 4)

CHAPTER 2

OPTIMIZED NEUTRON ACTIVATION ANALYSIS LABORATORY-BASED TOOL SYSTEM: PyNIC–DAKOTA[1]

2.1 Abstract

Accurate, optimized, effective and safe selection of neutron activation analysis (NAA) experimental parameters is essential in controlling the radiation dose to personnel while at the same time minimizing the generation of excessive radioactive products. This comes in competition with assuring that enough activity of an examined sample is produced in order to be able to measure targeted trace nuclei within the given laboratory framework including the available neutron source, sample preparation, and detector equipment. In this paper, the coupling of a NAA precalculator tool, PyNIC, with the optimization tool, DAKOTA, is described. This PyNIC–DAKOTA tool system is used to determine the optimal parameters for NAA performing fast yet accurate and effective optimization among many interrelated NAA parameters saving time and experimental efforts. Two examples using this novel PyNIC–DAKOTA tool system are presented in finding the optimal NAA parameters for detecting ^{60}Co from a sample of ^{59}Co and

[1] Ryan Schow and Tatjana Jevremovic, "Optimized Neutron Activation Analysis Laboratory-Based Tool System: PyNIC-Dakota", Submitted to *European Physical Journal - Nuclear Sciences and Technologies (EPJN)*, June 27, 2017.

detecting three target nuclides, ^{56}Mn, ^{139}Ba, and ^{42}K, from a standard reference sample of coal fly ash. The details of the optimization estimates are described in comparison to the real experimental values. The PyNIC–DAKOTA tool system shows expected agreement with actual NAA experiments and can be applied to any research reactor-based NAA facility.

2.2 Introduction

Neutron Activation Analysis (NAA) is a common nondestructive elemental concentration identification method [1]. NAA can measure the total amount of an element in a material irrespective of its chemical and physical state [2]. The advantages over other comparable methods are many: the samples can be liquids, solids, or powders, it is nondestructive, no special sample preparation is required leading to no reagent-introduced contaminants, multiple elements can be determined simultaneously, it has a high sensitivity to many trace elements, and is unaffected by the presence of organic materials [3]. Research nuclear reactors provide required neutron flux levels assuring higher sensitivity to detection of most elements and representing the most common neutron source used for the NAA. In applying the NAA, it is important to understand, assess and mitigate all associated ramifications of irradiating materials prior to placing the samples in a research reactor.

2.2.1 Minimizing radiation exposure and radiation dose

The International Atomic Energy Agency (IAEA) recommends that in order to satisfy the safety principles for research reactors, the doses from experiments are to be kept below the dose limits and as low as reasonably achievable (ALARA) [4]. In the United States, the Code of Federal Regulations [5] defines the ALARA as the "means of making every reasonable effort to maintain exposures to ionizing radiation as far below the dose limits as practical, consistent with the purpose for which the licensed activity is undertaken, taking into account the state of technology, the economics of improvements in relation to state of technology, the economics of improvements in relation to benefits to the public health and safety, and other societal and socioeconomic considerations, and in relation to utilization of nuclear energy and licensed materials in the public interest." Minimizing activation products is an important concern when 'large samples' are examined with the NAA (of interest to mineral mining industry, food industry, or material recycling industry) [3], [6].

2.2.2 Minimal detection level and lowest limit of detection

If the samples are not activated nearly enough, the trace elements will not be detected and the sample fine composition inaccurately determined, or they will stay below the minimal detection level (MDL) or the lowest limit of detection (LLD). A common method to estimate the minimum detectable activity (MDA) is using Currie's relation [7]:

$$MDA = \frac{\left(2.71+4.65\sqrt{B}\right)\times Decay}{\varepsilon\times b\times LT\times k\times q} \tag{2.1}$$

where:

$\left(2.71 + 4.65\sqrt{B}\right)$ – is Curries detection limit formula [7]

B – background counts under a gamma-ray peak of the nuclide of interest

$Decay$ – decay factor

ε – efficiency

b – abundance

LT - elapsed live time

k - 3700 dps/μCi

q - sample quantity

The constants in Eq. (2.1) are obtained by assuming a 5% error in detecting the targeted nuclide and a relative standard error of 10%. This methodology is effective when the gamma-ray background (counting statistical error) is the major interference. Several factors affecting the MDLs and associated with NAA are the sample size, sample irradiation time, neutron flux, detector efficiency, and signal to noise ratio (S/N). The MDL is proportional to the radiation detectors minimum detectable activity (MDA) which is the minimum detectable activity at a specified confidence level and depends on the counting device, counting times and background counting rate [8]. The MDA is usually the smallest quantity of a radioisotope, which can be detected with 95% confidence level. With these interrelated parameters, an optimization is well needed to select the best suited NAA parameters in thus assuring both minimizing the amount of radioactive elements produced and reducing as reasonable as achievable the radiation dose rates while ensuring that the activation of a sample is above the MDL.

In very recent years, at the University of Utah, we have established, highly organized and well-controlled steps in performing any experiment within the facility involving radiation that is generated at any level [9], [10]. The NAA and material irradiation experiments are the two main activities at the facility – used either for research or education and training of the students. Protocols and adherence to strict procedures for both are an absolute must as well as preservation of knowledge and recording of the data generated in such experiments [11]-[14].

2.2.3 Optimization of the NAA

Numerous facilities around the world for many decades have applied NAA as a common technique in analyzing samples of various sizes, types, contents, purposes, research, education, training, and investigations. Bode et. al [15] stated that the NAA technique has many adjustable experimental parameters that leads to the need for the experimental design of NAA to be optimized. Based on the extensive existing literature on NAA, and the known practices in many facilities world-wide, there has been no tool developed that can optimize the interrelated NAA parameters for its successful and well-optimized outputs while minimizing the exposure to radiation and generation of excessive waste [8], [16]. In this chapter, therefore, we describe our novel approach based on coupling our in-house code, *neutron interaction tool*, named PyNIC, with the well-known optimization tool, DAKOTA [17], in thus successfully optimizing the NAA experiments performed at our facility and maintaining an effective safety culture [13].

2.3 PyNIC: In-house python-based neutron interaction calculator

The Utah Nuclear Engineering Facility houses many advanced and modern laboratories in addition to one of few remaining TRIGA Mark I Reactors, abbreviated as UUTR; it is a pool type research reactor of hexagonal core geometry, licensed to operate at the maximum power of 100 kW_{th}. The UUTR is used for a variety of research, testing, and experiments since 1975. The NAA is one of the most frequent activities [18]. The UUTR has four different irradiation facilities that are used for various types of experiments (Figure 2.1). The irradiation facilities are located within the reactor core at different locations in thus providing different neutron flux levels, and corresponding neutron energy spectra properties with associated characteristics. The highest total neutron flux at 90 kW_{th} is in the central irradiator (CI) equal to 7.4×10^{12} $n/cm^2 \cdot s$, while the lowest flux at that same power level is in the thermal irradiator (TI) equal to 7.3×10^{11} $n/cm^2 \cdot s$. Once the specified power level is reached, the sample is placed into the indicated irradiation port for the predetermined irradiation time. The sample is then removed from the UUTR where the dose rate measurement is taken at 1 ft (30 cm) away from the sample/source. The distance of 1 ft aligns with U.S. NRC regulations that require radiation measurements to be taken at that distance from any source to determine posting and protection requirements [5]. Once irradiated, the sample is placed in the high-purity germanium (HPGe) detector where counting is conducted. Therefore, the following parameters must be determined prior to NAA: reactor power level, irradiation port in the UUTR (Figure 2.1), irradiation time of the sample within the port, sample mass, guessed sample elemental composition, and counting delay time between irradiation and counting. In order to accurately predict the activity and dose rates achieved from the planned NAA, a newly developed in-house Python-based neutron interaction calculator (PyNIC) was developed [19], [20]. Prior to the implementation of PyNIC, historically used calculators only accounted for the thermal flux of a neutron beam giving a rough approximation of the expected activity due to not accounting for the entire neutron energy spectrum [21],

[22].

The PyNIC algorithm is based on the physics of transmuting stable nuclei (parent isotope) present in a given sample when exposed to neutrons through mainly neutron capture interactions into new and radioactive nuclei (daughter isotope) that consequently emit gamma radiation. The gamma rays emitted due to the decay of the daughter isotope are unique, and thus used to identify the nuclei present in the sample. The PyNIC therefore requires the user's best estimate of the sample characteristics for predicting the daughter isotope's activity that in turns determines the dose rate that will be emitted from the daughter isotope. Therefore, the activity of a daughter isotope (in Bq) is calculated with:

$$A_D = m\left(\frac{N_A}{A_m}\right)A_{\%}\left(1 - e^{-\lambda_D t_{irr}}\right)e^{-\lambda_D t_{cdt}}\int_0^{\infty} dE\,\Phi(E)\sigma_p(E) \qquad (2.2)$$

where:

m – mass of sample (g)

N_A – Avogadro's Number

A_m – atomic mass (g/mole) of parent isotope

$A_{\%}$ – atomic abundance ratio of the parent isotope in the sample

λ_D – decay constant of daughter isotope (s^{-1})

t_{irr} – irradiation time (s)

t_{cdt} – counting delay time (s)

$\Phi(E)$ – neutron flux at energy E (n/(cm^2•s))

$\sigma_p(E)$ –radiative capture cross-section of the parent isotope for neutrons with kinetic energy E (cm^2)

The PyNIC algorithm accounts for a wide neutron energy spectrum in order to attain a higher level of accuracy in predicting neutron activation of a sample, and also includes the database on prompt gamma ray emissions as a result of neutron capture. The neutron flux is known in each of the UUTR irradiation facilities based on the comprehensive MCNP6 and AGENT code models [23]-[26]. The PyNIC database includes neutron capture cross-sections, selected inelastic scattering cross-sections, and 23 selected fission cross-sections values based on pointwise ENDF-VII at 300 K [27]. The activation products and immediate gamma emissions of a sample are straightforwardly predicted with PyNIC simulation.

Once the activation of the sample is calculated with PyNIC, there is a direct link for licensed MCNP-users to a MCNP6 UUTR model inclusive of a sample's decay with a corresponding gamma spectrum expected to be measured with the HPGe detector in the laboratory. A user–friendly graphical user interface (GUI) allows for a simple selection of the required input parameters: sample mass, irradiation time in the selected UUTR irradiation port, counting delay time (sample decay time), UUTR (research reactor) power, and the choice of nuclides expected to be contained / activated within the sample which are of interest to the user to detect. The snap shot of the input GUI is shown in Figure 2.2.

The output of the PyNIC simulation is generated as an *easy-to-read* text file report (an example is shown in Figure 2.3) listing the activity of the targeted nuclides and the associated dose rate at 1 ft (30 cm) from the sample when it is removed from the reactor tank as shown in Figure 2.4.

As shown in Figure 2.5, the steps required to determine the best NAA parameters at the UUTR facility include:

1. Estimate the NAA input parameters (i.e., sample mass, irradiation time, irradiation port, reactor power level, and counting delay time): this can be done by starting with similar historical NAA experiments conducted at the UUTR or estimate the best guess values.
2. Input the NAA parameters into PyNIC (example as shown in Figure 2.2)
3. PyNIC produces a report with the values of the activity and dose rate for the nuclides of interest (example as shown in Figure 2.3).
4. If the activity of the targeted nuclide is above MDL and the dose rate is below limits established for the facility, the NAA can be performed.
5. If nonsatisfactory results are obtained, the steps 2 to 4 are repeated.

2.4 DAKOTA system

2.4.1 DAKOTA applications

DAKOTA, a Design Analysis Kit for Optimization and Terascale Applications, is developed and maintained by Sandia National Laboratories [17]. The DAKOTA software is open source and thus readily available for use and implementation. DAKOTA offers a common set of optimization tools for engineers solving structural analysis and design problems and includes methods for parameter estimation, global sensitivity and variance analysis, uncertainty quantification, and verification, as well as meta-level strategies for surrogate-based optimization, hybrid optimization, and optimization under uncertainty. An important advantage in using DAKOTA with other codes and methods is access to a wide range of iterative capabilities through a single and simple interface. Some examples of recent applications of DAKOTA's uncertainty solvers and its use in the design of experiments aimed at improving nuclear safety are as follows:

- The nuclear fuel performance code, BISON, was coupled with DAKOTA to perform uncertainty and sensitivity analysis on fission gas behavior, and thus lead to improved safety in ensuring nuclear fuel is not compromised during transients [28]. The complex behavior of fission gases has a significant impact on the thermo-mechanical performance of nuclear fuel and needs to be accurately predicted. Five fission gas behavior parameters were selected to determine how the uncertainty of those parameters impacts the fission gas release and volumetric swelling outcomes of BISON calculations. DAKOTA's sensitivity analysis method, orthogonal array sampling (OAS), was utilized for estimating the main effects. Main effects include a sensitivity analysis method, which identifies the input variables that have the most influence on the output. The five parameters of the fission gas behavior, temperature, grain radius, intra-granular gas atom diffusion coefficient, intra-granular resolution parameter, and grain-boundary diffusion coefficient were varied within ranges representative of the relative uncertainties and consistent with published literature. Coupling DAKOTA with BISON allowed demonstration of the significant deviation in results of the fission gas release and cladding diametral strain during power transients with the current uncertainty of specific parameters involved. Fission gas behavior calculations can be improved by better characterization of the intra-granular gas atom diffusion coefficient because it was determined that this parameter's uncertainty has a large impact on the calculations of BISON. This will lead to improved safety of reactor fuel use due to the improved calculations on fuel transients.

- To ensure used nuclear fuel is kept within the safety limits during dry storage conditions, the Best Estimate Plus Uncertainty (BEPU) code FRAPCON-3xt was coupled with DAKOTA to perform uncertainty analysis [29]. When nuclear fuel is placed in dry storage, the stress on the fuel cladding is the main damaging mechanism postulated for failure and needs to be clearly understood to enhance safety during the long-term dry storage of nuclear fuel. An analytical approach based on thermo-mechanical predictions for cladding hoop stress in dry storage conditions was performed with FRAPCON-3xt [30]. The precision of this tool can be limited by the input uncertainties. In order to assess nuclear safety, the upper bound of the cladding hoop stress uncertainty needs to be determined so that the remaining safety margin can be determined. DAKOTA's uncertainty analysis method, Latin Hypercube sampling, was deployed in determining the upper bound of the cladding hoop stress given the uncertainties of the inputs to FRAPCON-3xt such as ten fuel rod design variables and in-code fuel models. The Latin Hypercube method sampled probability distribution functions and 3000 samples were taken. It was found that the uncertainty in fission gas release is the most influencing factor with regards to cladding hoop stress, so improvements in fission gas release modeling will enhance accuracy and safety of dry fuel storage. The allowed fuel burnup and maximum storage temperature to ensure fuel integrity during storage was also determined. Nuclear fuel storage safety was enhanced by coupling FRAPCON-3xt with DAKOTA.

- Reactor safety is dependent upon correct, accurate, and timely modeling of the physics within a nuclear reactor and its nuclide depletion. In order to determine the depletion of the nuclide inventory in a reactor, loose coupling of two physics codes, a steady state neutron transport code or diffusion calculation with a time-dependent nuclide depletion calculation, is used and called lattice physics depletion. The stepsize of the lattice physics depletion algorithms impacts both the solution accuracy and computational time. DAKOTA was utilized in developing an adaptive stepsize selection algorithm to improve accuracy and reduce computational time when using the lattice physics depletion methods [31]. DAKOTA's Latin Hypercube sampling algorithm was used to efficiently parameterize the stepsize controller so that a general controller could determine the optimal lattice depletion stepsize. Due to DAKOTA's sampling, it was found that the initial stepsize affects the total number of steps taken (reduced time), while only introducing a few pcm additional error. This in turn will lead to more efficient calculations of reactor core depletion and improved reactor safety models.

2.4.2 DAKOTA EA optimization algorithms

The DAKOTA optimization evolutionary algorithm (EA) called single-objective genetic algorithm (SOGA), is used in coupling with PyNIC. The SOGA is a global optimization method that supports general constraints and a mixture of continuous and discrete variables. The more common type of variables used in engineering applications are of the continuous type. Continuous variables may assume any real value within the bounds input by the user (e.g., sample mass is bounded by 0.05-50.0 gm). In the case of NAA, such values can be sample mass, irradiation time, or counting delay time. Engineering design problems also contain discrete variables such as types of materials. Discrete variables may involve a set of integer values (e.g., reactor power can be 30, 70, or 90 kW), a range of consecutive integers (e.g., reactor power can be any integer between 10 and 20 kW), a set of string values (e.g., reactor power and irradiation port can be 'PI_10', TI_50', or 'FNIF_90'), or a set of real values (e.g., reactor power can be identically 10.9, 22.5, or 79.1 kW). Discrete variables used with PyNIC are the experimental port and power level of the reactor as a set of string values such at PI_50 (Pneumatic Irradiator at 50 kW).

SOGA is based on Darwin's theory of survival of the fittest, which means the set of continuous and discrete variables that give the most optimal outcome will continue to be replicated and mutated for future generations or solutions. The SOGA starts with a randomly selected population of design points in the parameter space, where the values of the design variables form a "genetic string," similar to DNA in a biological cell, that distinctively characterizes each objective function. The objective function is the calculation or outcome of the specific code, such as PyNIC, that the SOGA is trying to minimize. The SOGA then follows a series of generations, where the best objective functions in the population are considered the most "fit" and are allowed to endure and replicate. This method mimics the evolutionary process by utilizing the mathematical analogs of processes such as natural selection, breeding, and mutation [32].

The basic steps of the SOGA include:

1. Initialize the population.

2. Calculate the values of the objective function for the initial population.
3. Perform the following loop until convergence or stopping criteria are reached:
    a. Implement crossover.
    b. Perform mutation.
    c. Evaluate the new population.
    d. Consider the fitness of each member in the population.
    e. Replace the population with members selected to continue in the next generation.
    f. Check for convergence.

An example of the SOGA optimization is here demonstrated by trying to generate a particular character string, for example, "PYNIC." Each of the possible solutions in the population will be a string of fixed-length that is 5 characters long. The possible characters in a string are one of the 26 valid characters (upper case letters "A" to "Z"). To determine the fitness or objective function of each solution, a candidate solution will receive one point for each position in the string that has the correct character (i.e., 1 point is given for the character "P" in the first position or 1 point is given for the character "C" in the last position). This gives the maximum possible fitness score of 5 if all character's spell "PYNIC."

The SOGA Step 1 is to randomly generate the initial population. The user can select any size population that is desired. For this example, each population is size 10. The following list of 10 iterations could be a possible initial population with their objective function value in brackets (Step 2):

1. IPSCN (0)

2. PQWRS (1)
3. YKRBR (0)
4. LDDLI (0)
5. UWALP (0)
6. OGNIV (2)
7. ABBRM (0)
8. OXPCQ (0)
9. LBBOY (0)
10. SPBJC (1)

The list above shows that iteration number 6 is the best with a fitness score of 2 with 2 characters out of the 5 in the correct position that match the target string. To perform the Step 3, the iterations are selected based on their fitness to create a new generation and be the "parents." SOGA uses an "elitist" replacement type that creates the new population from the best individuals in the current population. The crossover is implemented by a randomly selected crossover point (Step 3. a.) as follows:

Parent 1: PQWRS

Parent 2: OGNIV

Offspring 1: PQNIV

Offspring 2: OGWRS

In this case, the crossover was implemented after the second character. The offspring 1 now has an improved fitness score of 3. This is a demonstration of how crossovers can lead towards better solutions. However, looking at the initial population, if the algorithm only uses crossover, the best solution would still not be able to achieve the string “PYNIC.” This can be improved by increasing the population size. Another part of the process also can lead to the correct solution, which is mutation (Step 3b.). Mutation is implemented by modifying each character in a parent string according to some probability, say 0.03 or 0.06. Those numbers are the probability that any single parent will be changed by mutation. By applying mutation to a set of offspring produced in crossover, sometimes new correct characters can be introduced into new positions (such as the Y in the second character). After repeating this process for many iterations, the algorithm will converge to the desired “PYNIC” string.

The SOGA’s ability to handle both the continuous and discrete variables is important for coupling with PyNIC. PyNIC has both continuous variable inputs (sample mass, irradiation time, and counting delay time) as well as discrete variable inputs (UUTR irradiation port and power level).

2.5 The PyNIC-DAKOTA system

The PyNIC-DAKOTA system’s flow chart is given in Figure 2.6. The overall process starts with a DAKOTA input file that initiates an optimizer algorithm, SOGA, which iterates the PyNIC solver. This begins by DAKOTA generating an input parameters file that is then preprocessed to initiate PyNIC. PyNIC executes its calculations for activity and dose rate and is postprocessed into a file for the DAKOTA SOGA to utilize in the optimization calculations. This process is then repeated until an optimal solution is obtained.

In general, the DAKOTA coupling system is initiated with a DAKOTA input file containing six different blocks defined as:

- *Environment block:* defines general DAKOTA settings such as graphical and tabular data, output settings (this block is optional);
- *Method block:* specifies which iterative method is used such as optimization, uncertainty quantification, calibration, or parameter studies.
- *Model block:* is optional and provides the logical unit for determining how a set of variables are mapped through an interface into a set of responses when needed by an iterative method;
- *Variables block:* stipulates the number, type, and characteristics of the parameters that will be varied.
- *Interface block:* is used to map variables into responses as well as specifics on how DAKOTA will pass data to and from the code like PyNIC or any other code in which DAKOTA is communicating with.
- *Responses block*: specifies the types of data that the interface will return to DAKOTA.

For the coupling of PyNIC and DAKOTA, the *method, variables, and interface* blocks are used to provide the key information and execution commands as follows:

- *Method* block: provides the connection to the SOGA iterative method where the convergence criteria, crossover type, and mutation type are specified. The convergence criteria controls when the SOGA will terminate its iterations.
- *Variables* block: splits the variables into continuous and discrete variables. The PyNIC requires one discrete and three continuous variables as shown in Table 2.1. The irradiation ports and power levels are specified in the PyNIC. DAKOTA interfaces with the PyNIC, by communicating through the file system

accomplished through the reading and writing of parameters and results in the files labeled "DAKOTA Input Parameters" and "DAKOTA Optimization Parameters" as detailed in Figure 2.6. An example of the "DAKOTA Input Parameters" file is shown in Figure 2.7.

- *Interface* block: specifies the simulation code, PyNIC that will be used to map variables into responses as well as details on how DAKOTA passes data to and from PyNIC. A pre- and postprocessing environment is needed to convert the "DAKOTA Input Parameters" file (Figure 2.7) and the "DAKOTA Optimization Parameters" file into the corresponding formats required by PyNIC and DAKOTA.

PyNIC determines the activity of the targeted nuclei in the sample from the selected variables based on Eq. (2.2). The objective of the PyNIC – DAKOTA system is to minimize the activity of targeted nuclei after the neutron activation to be near the MDL value. In order for DAKOTA to determine the input parameters needed to achieve the MDL of targeted nuclei, the PyNIC calculated activity is inserted into an objective function (Obj. Fn) given with:

$$\mathrm{Obj.\,Fn} = \left|\mathrm{Calculated\ Activity}_{\mathrm{PyNIC}}\left(\frac{\mu\mathrm{Ci}}{\mathrm{g}}\right) - \mathrm{MDL}\left(\frac{\mu\mathrm{Ci}}{\mathrm{g}}\right)\right| \quad (2.3)$$

The objective function is needed to optimize a value near MDL and is the output that the SOGA is minimizing.

The SOGA is minimizing the absolute difference between the specific activity and the MDL. The DAKOTA SOGA iterates until a convergence criteria specified by the user is met. Once this is complete, an output file is generated providing the best combinations of variables for a given input. In this case that would be the best set of parameters for the neutron activation experiment to achieve minimal activation of sample with a required level of detection. This improves nuclear safety in the facility by minimizing unnecessary activation of products and reduces dose.

2.6 Benchmark tests of the PyNIC-DAKOTA system

2.6.1 Determining the optimal NAA parameters for $^{59}Co \rightarrow ^{60}Co$

An example to test the PyNIC–DAKOTA system in determining the optimal parameters to conduct NAA of pure ^{59}Co in the UUTR and measure ^{60}Co near its MDL is described. The input parameters used are given in Table 2.2 for a 100% mass abundant sample of ^{59}Co. The MDL value was 0.02 μCi/g. Based on the variable inputs as described in Table 2.2, the SOGA generated an initial population of 50 iterations. PyNIC determined the objective function for each of the 50 iterations. SOGA then performed the crossover and mutation producing a new population that includes members from the previous generation and the new crossover and mutation members. This process was repeated until the inputted convergence criterion of 10^{-5} was achieved on the objective function from Eq. (2.3). The SOGA converged after 79 different populations of 50 iterations with selected portions of the 79 populations from the beginning, middle, and end as shown in Table 2.3. This included 1,000 different iterations at convergence using the SOGA method. Table 2.3 shows that the SOGA selected variables that PyNIC utilized in each iteration and the resulting objective function. SOGA minimized the objective function, which can be seen overall reducing as the number of iterations increases. The reason for sometimes larger values of the objective function in higher iterations is due to the mutation that the SOGA implements.

The output file from DAKOTA for determining the optimal parameters for NAA of pure ^{59}Co is given in Figure 2.8 listing the best parameters. The optimal solution is achieved at iteration 947 with the parameters as seen in both Table 2.3 and Figure 2.8. This example shows how the PyNIC-DAKOTA system can "advise" an experimenter who wanted to measure ^{60}Co utilizing NAA at the UUTR starting with pure ^{59}Co, on the best selected parameters: the mass of 0.669 gm of ^{59}Co should be placed in the TI facility at a reactor power of 1 kW_{th} for 1.5 min with a counting delay time of 21.6 min. Using the selected parameters, PyNIC projects an activity level of 0.0194 μCi/g of ^{60}Co that will be created. If the PyNIC calculated activity level is placed into Eq. (2.3) with 0.02 μCi/g MDL, the objective function of 0.0006 is obtained as seen in Figure 2.8 under "Best objective function."

2.6.2 Comparison of PyNIC-DAKOTA system with the experimental data for the NAA of coal fly ash standard samples

A series of irradiation experiments in the UUTR were performed using coal fly ash standards (1633c) from the National Institute of Standards and Technology (NIST) [33]. All irradiations of the coal fly ash were for 2 min in the TI of the UUTR (Figure 2.1). There are many variables involved with this process and it was determined from previous NAA that the coal fly ash samples would only need to be irradiated in the TI at lower power levels to be near the MDL for the target nuclides of interest. Table 2.4 shows specifics of the coal fly ash irradiations performed at the UUTR in the past. After irradiation, the activity of the coal fly ash was measured using a high-purity germanium (HPGe) detector. The coal fly ash samples were placed on the detector inside of a lead and copper shield as shown in Figure 2.9 and counted for a total of 10 min each. The Canberra GENIE software was used to identify the isotopes. Coal fly ash is made of many different nuclides, however, the only nuclides used to test the PyNIC-DAKOTA system are ^{56}Mn, ^{139}Ba, and ^{42}K.

It can be seen in Table 2.4 that the ^{56}Mn was detected in all cases, that the ^{139}Ba was not detected until the UUTR power level of 10 kW_{th}, and that the ^{42}K was not detected until the UUTR power level of 30 kW_{th}. The MDLs for the targeted nuclides were obtained from the capabilities of the detection equipment used at UNEP as seen in Figure 2.9. The MDLs input into the PyNIC-DAKOTA system were 0.04 μCi/g for ^{56}Mn, 0.03 μCi/g for ^{139}Ba, and 0.19 μCi/g for ^{42}K. The PyNIC-DAKOTA system is applied with the goal to find the optimal NAA input parameters to detect ^{56}Mn, ^{139}Ba, and ^{42}K in a fly ash standard sample at the UUTR. The PyNIC-DAKOTA system can only target one nuclide at a time, so three separate PyNIC-DAKOTA system runs were conducted, one for each of the three targeted nuclides of ^{56}Mn, ^{139}Ba, and ^{42}K. The variable input parameters into the PyNIC-DAKOTA system are given in Table 2.5. PyNIC input also requires the percent mass abundance of the targeted nuclides. The percent mass abundance of the standard coal fly ash samples' targeted nuclides are 0.024% for ^{55}Mn, 0.125% for ^{41}K, and 0.081% for ^{138}Ba; these values are obtained from the certificate of analysis from the National Institute of Standards and Technology (NIST), [33].

2.6.2.1 Determining the optimal NAA parameters for ^{56}Mn in coal fly ash in the UUTR

The PyNIC-DAKOTA system included 1000 iterations at convergence using the SOGA method to determine the optimal parameters for ^{56}Mn NAA-based detection. Table 2.6 shows the SOGA selected variables that PyNIC utilized in each iteration and the resulting objective functions. Table 2.6 displays that SOGA is minimizing the objective function along with various mutations that periodically cause the objective function to increase. The SOGA implements mutations in order for the algorithm to avoid concentrating on a local minimum. This ensures that the entire variable range is explored. Sometimes when the mutations occur they result in less fit solutions and the less fit solutions do not get replicated or continued in the process.

The results from the PyNIC-DAKOTA system for determining the optimal parameters of ^{56}Mn for NAA of coal fly ash are given in Figure 2.10. The best NAA parameters were obtained at iteration 797 as seen in Table 2.6 and Figure 2.10. The PyNIC-DAKOTA system recommends that a mass of 0.076 gm of coal fly ash should be placed in the TI facility at a reactor power of 1 kW_{th} for 2.2 min with a counting delay time of 30.5 min to find ^{56}Mn in coal fly ash near its MDL of 0.04 μCi/g. The experimental results for ^{56}Mn had a range of 0.161-0.208 gm of coal fly ash placed in the TI at a power of 1 kW_{th} for 2.0 min with a counting delay time of 8.5-11.0 min which resulted in measured ^{56}Mn activities of 0.023 to 0.042 μCi/g. The PyNIC-DAKOTA system solutions sample mass is lower than the experimental results, but with the slightly longer irradiation time of 2.2 min compared to 2.0 min compensates for this and demonstrates that a slightly smaller sample could be used, thus reducing dose.

2.6.2.2 Determining the optimal NAA parameters for

^{139}Ba in coal fly ash in the UUTR

The PyNIC-DAKOTA system provided the answer in 1,000 iterations to determine the best parameters for finding ^{139}Ba in coal fly ash. Table 2.7 summarizes the NAA parameters for the given iterations and the PyNIC resulting objective function that the SOGA is minimizing.

The PyNIC-DAKOTA system successfully found the ideal NAA parameters for determining ^{139}Ba in coal fly ash as displayed in Figure 2.11. The optimum solution was found at the 876th iteration. The recommended solution from the PyNIC-DAKOTA system for determining ^{139}Ba from coal fly ash is for a sample mass of 0.157 gm and the TI facility with a UUTR power of 10 kW_{th} for 2.3 min of irradiation with a counting delay time of 44.3 min (Table 2.7 and Figure 2.11). This is compared to the experimental results in the UUTR of sample mass 0.131 – 0.162 gm in the TI with a power of 10 kW_{th} for 2.0 min and counting delay times of 27.0 – 33.0 min and a measured activity of ^{139}Ba of 0.036 – 0.046 μCi/g. The ^{139}Ba experimental results agree closely with the PyNIC-DAKOTA system.

2.6.2.3 Determining the optimal NAA parameters for

^{42}K in coal fly ash in the UUTR

Table 2.8 shows the sample parameters used in the PyNIC-DAKOTA system in order to determine the best NAA parameters in accurately finding ^{42}K in coal fly ash and the system optimizing objective function.

Figure 2.12 shows the PyNIC-DAKOTA system output file with the best NAA parameters for the investigations of ^{42}K in coal fly ash. The PyNIC-DAKOTA system provided that the ideal set of NAA parameters to detect ^{42}K is at iteration 932: 0.283 gm of coal fly ash irradiated in the TI facility at the UUTR power of 30 kW_{th} for 1.9 min and with the counting delay time of 17.0 min. The experimental results for ^{42}K were 0.118 – 0.165 gm of coal fly ash in the TI at 30 kW_{th} for 2.0 min with a counting delay time of 44.0 – 61.0 min. This demonstrates the ability of the algorithm to find the optimal parameters for conducting NAA to find ^{42}K in coal fly ash at the UUTR as shown in Figure 2.12 and Table 2.8.

2.6.2.4 Benchmark analysis

The PyNIC-DAKOTA system successfully determined the optimal parameters for detecting ^{56}Mn, ^{139}Ba, and ^{42}K in a coal fly ash standard sample utilizing the UUTR and UNEP facilities. Table 2.9 summarizes the PyNIC-DAKOTA system data in comparison to the experiment. The PyNIC-DAKOTA system optimization resulted in the selection of the same irradiation port and power levels that have been used in the experiment. Also, the irradiation times determined by the PyNIC-DAKOTA system of approximately 2 min were similar to the UUTR NAA experiment.

The UUTR NAA experimental values are close to optimal values because the coal fly ash samples were irradiated at varying power levels and sample sizes until the nuclides of interest, ^{56}Mn, ^{139}Ba, and ^{42}K, were detected. From historical experience of coal fly ash irradiations, it was determined that 2 min irradiations are adequate and commonly used to measure those nuclides of interest and that is why the irradiation time was held constant during this process.

The largest differences between the PyNIC-DAKOTA system and the experiment are in the counting delay times. The counting delay times can be used by the PyNIC-DAKOTA system to fine adjust the level of the activity measured in the detector depending on the properties of the nuclide of interest. If the nuclide has a short half-life, the counting delay time has a greater impact on the nuclides resulting activity whereas the activity from a nuclide with a long half-life has little adjustment with changes in counting delay time. ^{56}Mn, ^{139}Ba, and ^{42}K have half-lives of 155, 83, and 742 min, respectively, which would be considered short half-lives with the timeframes of 10-100 min. The PyNIC-DAKOTA system resulting objective function values when nearing the optimal solution are in the range of 10^{-4} to 10^{-6} as seen in the right-hand columns of Tables 2.6-2.8. The algorithm uses the counting delay time as a fine-tuning variable to adjust the small values of the objective function. Experimentally, the adjustment of the counting delay time is not used for targeting a specific activity level measured. This most likely explains the differences in counting delay times between the PyNIC-DAKOTA system and the experiment.

2.7 Conclusion

Neutron activation analysis (NAA) is a commonly used tool by many researchers and scientists to determine the elemental properties of various samples. Regulations, good practices, and enhanced nuclear safety cultures require that facilities try to activate as little materials as possible and maintain ALARA. This is in competition with activating target nuclides to high enough activities to also measure the activity with given laboratory equipment and procedures (≥MDL). It is proposed that the optimal NAA parameters such as sample size, irradiation time, neutron flux (reactor port and power level), and counting delay time can be determined prior to the actual conduct of the NAA using the coupling of an optimization code, DAKOTA, with a neutron interaction calculator, PyNIC. The PyNIC-DAKOTA tool system was successful in determining the optimal experimental parameters for conducting NAA at research reactors. This concept was demonstrated by comparing the PyNIC-DAKOTA system recommended experimental parameters with actual NAA that was conducted at the UUTR. Specifically, this was completed by determining the optimal parameters to conduct NAA of pure ^{59}Co in the UUTR and measure ^{60}Co near its MDL and of a standard coal fly ash in the UUTR to determine ^{56}Mn, ^{139}Ba, and ^{42}K. The results indicated that the PyNIC-DAKOTA system was thorough and accurate in finding the optimal experimental parameters for NAA with slight variations from the experiments.

The PyNIC-DAKOTA system has been shown to enhance the nuclear safety at the facility by minimizing dose and radiation waste products. This is similar to other examples of those implementing DAKOTA with various codes in improving nuclear safety [28], [29], [31]. This method could be utilized at any research reactor facility to optimally determine the parameters for conducting NAA and improve the nuclear safety. The items needed to complete this work at a different facility would be the neutron flux in the research reactor's irradiation facilities by using a complete MCNP6 model of the reactor core and irradiation facilities and the MDL for the laboratory equipment used to measure the nuclide of interest.

Future work includes continued benchmarking of the PyNIC-DAKOTA tool system to additional NAA experiments including a variety of materials and activities.

Other potential improvements would be in making a more user-friendly interface for the PyNIC-DAKOTA tools system, possibly a graphical user interface (GUI), so that end users will not need to have an understanding and knowledge of the python coding and DAKOTA input files.

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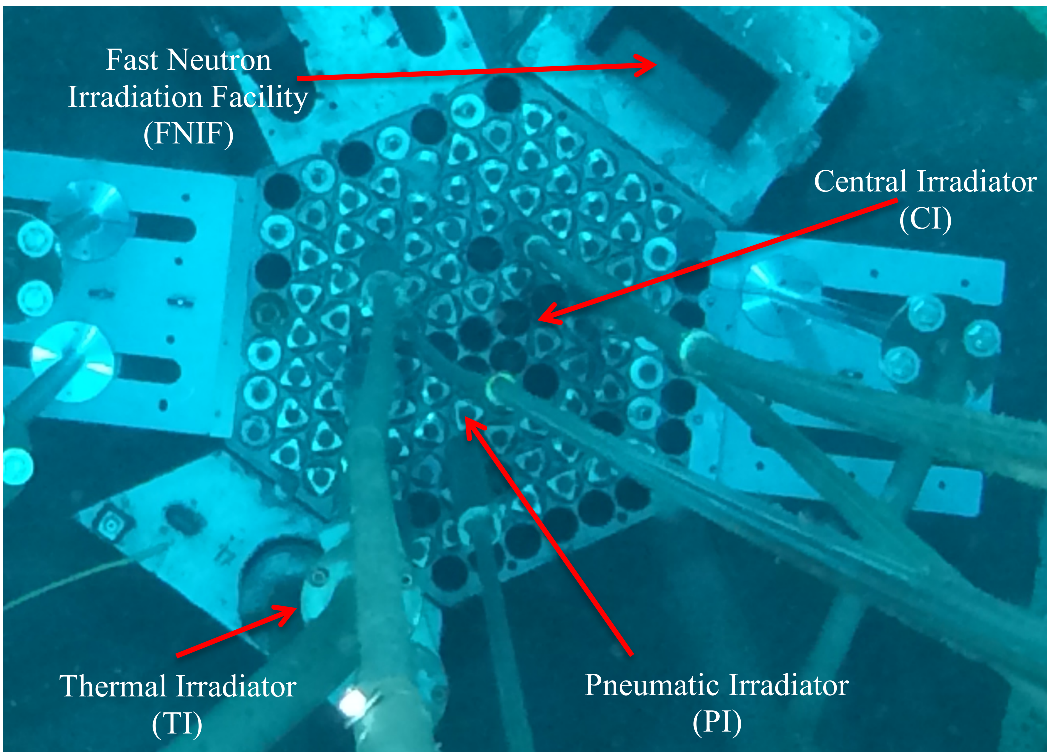

Figure 2.1: UUTR core and four irradiation ports - total neutron flux ranges from highest in CI=7.4x1012 n/(cm^{2}s) to lowest in TI=7.3x1011 n/(cm^{2}s)

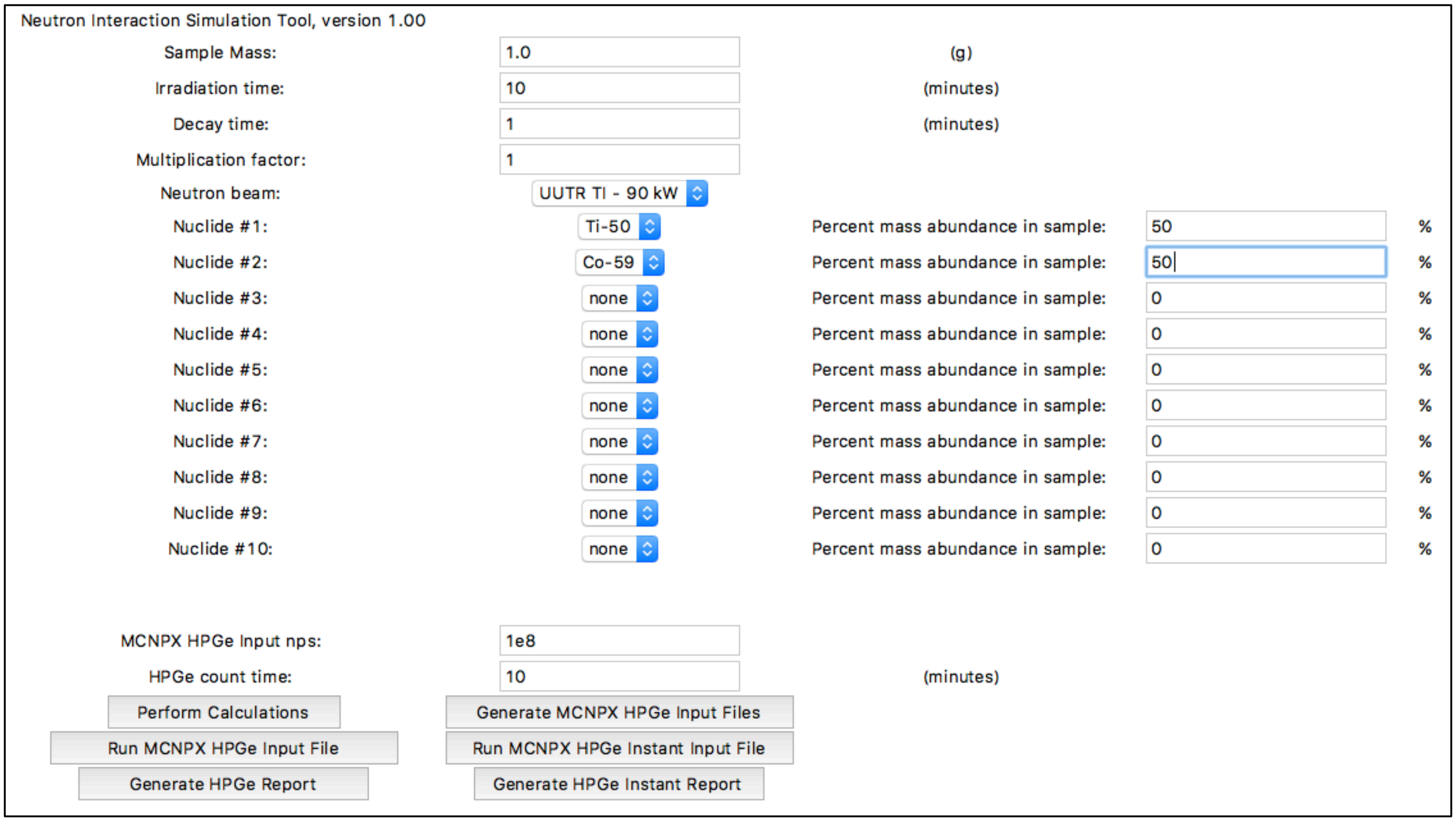

Figure 2.2: PyNIC graphical user interface (GUI): interactive selection of input parameters

```
==============================================================
UNEP NAA Calculator Version 1.01B 11-August-2014
==============================================================
Sample Mass: 1.0 g
Irradiation Time: 10.0 min
Decay Time: 1.0 min
Neutron Beam: UUTR TI - 90 kW
Table 1. Activation Products
============================================================================
Nuclide          Activity (mCi)       Activity (uCi/g)     Half-life (minutes)
============================================================================
Ti-51            6.15e+00             6.15e+03             5.76e+00
Co-60            4.52e-03             4.52e+00             2.77e+06
none             0.00e+00             0.00e+00             0.00e+00
none             0.00e+00             0.00e+00             0.00e+00
none             0.00e+00             0.00e+00             0.00e+00
none             0.00e+00             0.00e+00             0.00e+00
none             0.00e+00             0.00e+00             0.00e+00
none             0.00e+00             0.00e+00             0.00e+00
none             0.00e+00             0.00e+00             0.00e+00
none             0.00e+00             0.00e+00             0.00e+00
Total            6.15e+00

Table 2. Calculated Dose
==============================================================
Nuclide          Dose Rate (mrem/hr)
==============================================================
Ti-51            4.03e+01
Co-60            1.18e-01
none             0.00e+00
none             0.00e+00
none             0.00e+00
none             0.00e+00
none             0.00e+00
none             0.00e+00
none             0.00e+00
none             0.00e+00
Total            4.05e+01
```

Figure 2.3: PyNIC output text file: input parameters are summarized in the top (refer to Figure 2.2) - the two targeted nuclides, Ti-51 and Co-60, and their activities and half-lives are provided in Table 1 of Figure 2.3 and the dose rates from these targeted nuclides are given in Table 2 of Figure 2.3

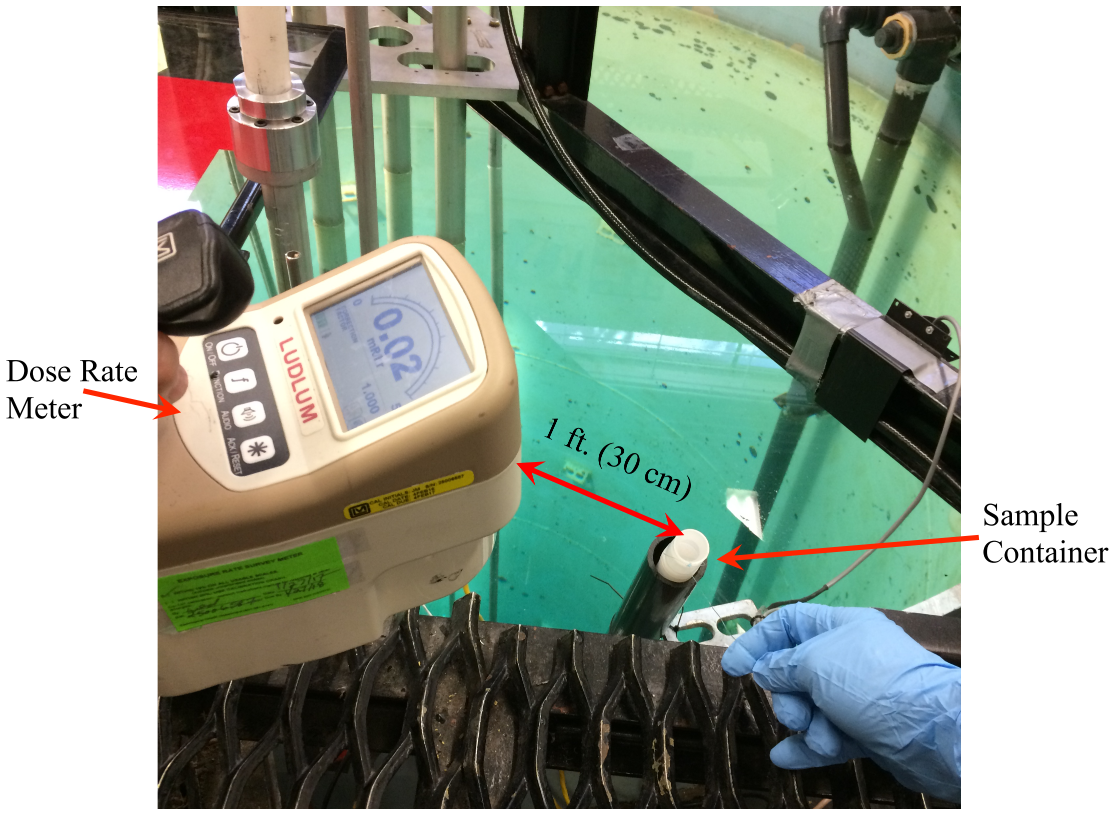

Figure 2.4: Sample dose rate measurement when removed from the UUTR

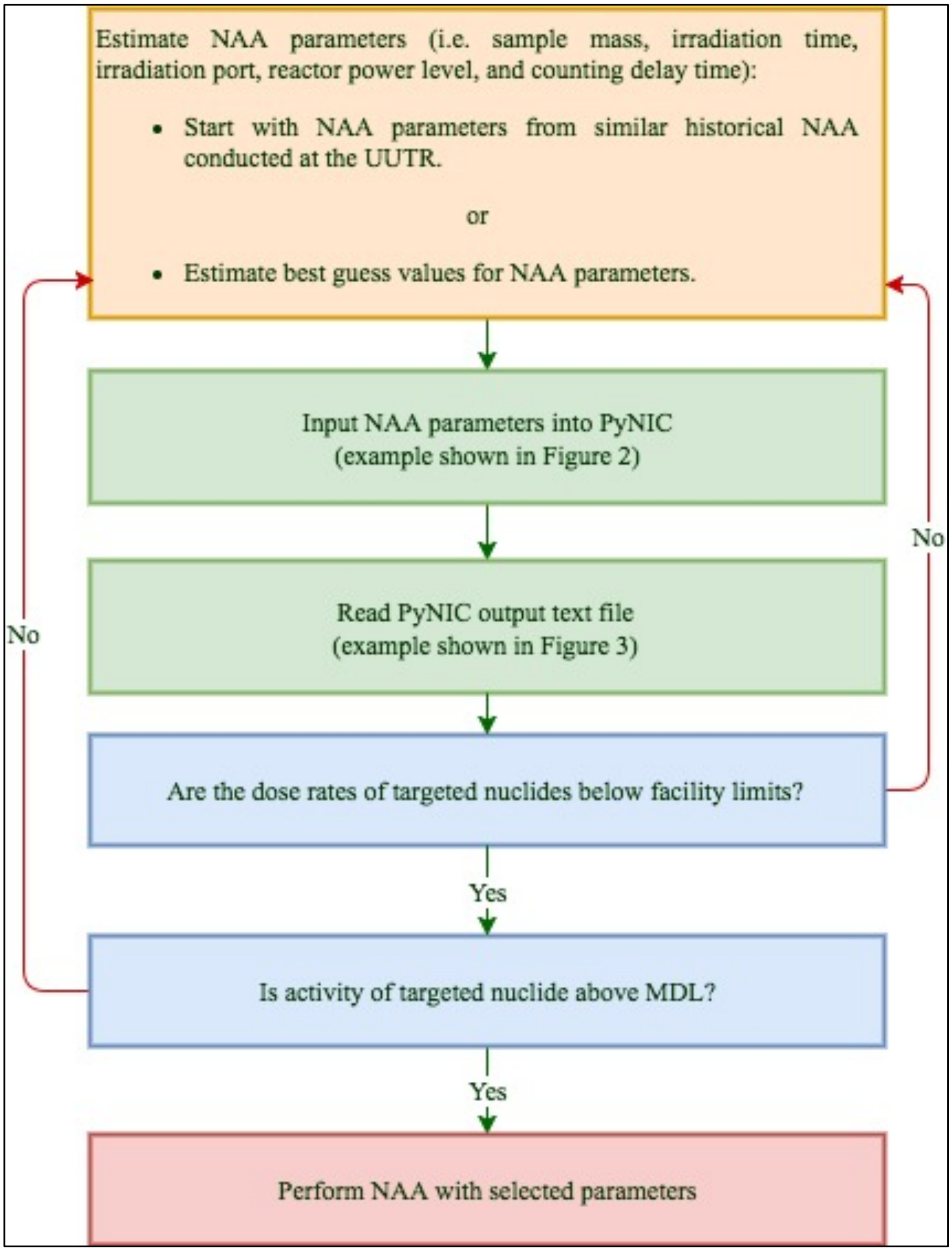

Figure 2.5: Steps taken in determining the best NAA parameters (at the University of Utah Nuclear Engineering Facility)

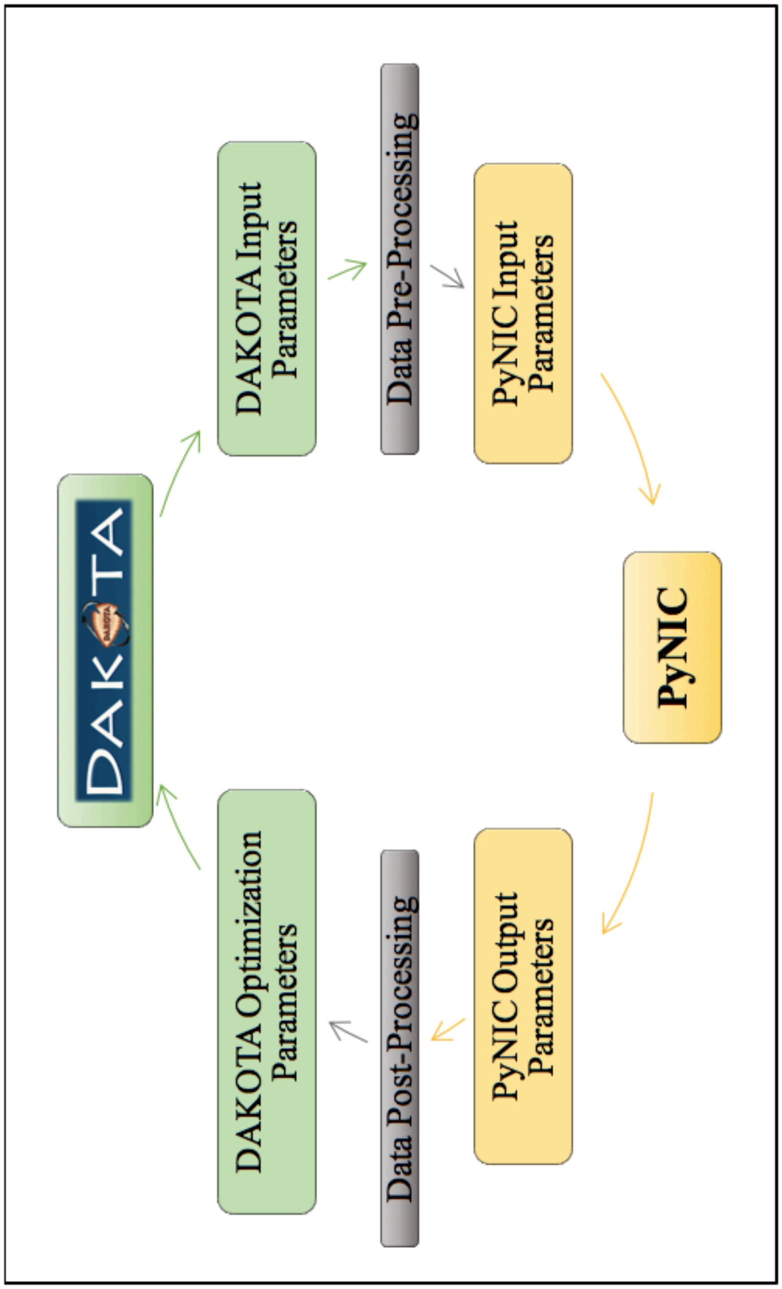

Figure 2.6: PyNIC–DAKOTA system

```
                    4 variables
1.309222992362012e+00 mass
1.261058398751682e+02 IrrTime
9.657982307286985e+02 DecayTime
                PI_10 irradPort
                    1 functions
                    1 ASV_1:obj_fn
                    3 derivative_variables
                    1 DVV_1:mass
                    2 DVV_2:IrrTime
                    3 DVV_3:DecayTime
                    0 analysis_components
                    1 eval_id
```

Figure 2.7: Example DAKOTA input parameters file

```
<<<<< Function evaluation summary: 1000 total (1000 new, 0 duplicate)
<<<<< Best parameters          =
                      6.6890330621e-01 mass
                      1.5025938174e+00 IrrTime
                      2.1553347873e+01 DecayTime
                                  TI_1 irradPort
<<<<< Best objective function  =
                      6.0648099782e-04
<<<<< Best data captured at function evaluation 947


<<<<< Iterator soga completed.
<<<<< Environment execution completed.
DAKOTA execution time in seconds:
  Total CPU        =    3.69056 [parent =    3.69054, child =    1.7e-05]
  Total wall clock =    205.353
```

Figure 2.8: PyNIC-DAKOTA system output file for determining the optimal parameters for $^{59}Co \rightarrow ^{60}Co$ NAA in the UUTR

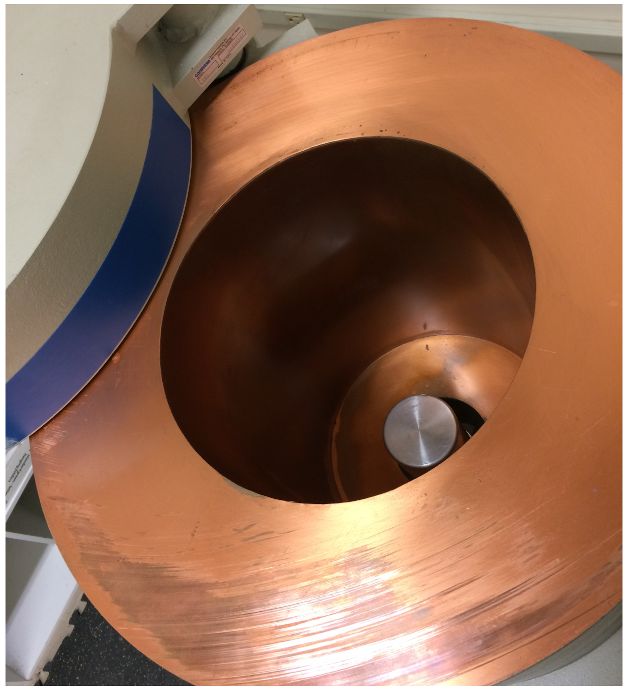

Figure 2.9: HPGe detector with Canberra lead and copper shielding at the University of Utah Nuclear Engineering Facility

```
<<<<< Function evaluation summary: 1000 total (1000 new, 0 duplicate)
<<<<< Best parameters          =
                      7.6008352649e-02 mass
                      2.1939662831e+00 IrrTime
                      3.0529046392e+01 DecayTime
                                  TI_1 irradPort
<<<<< Best objective function  =
                      1.4438722167e-04
<<<<< Best data captured at function evaluation 797


<<<<< Iterator soga completed.
<<<<< Environment execution completed.
DAKOTA execution time in seconds:
  Total CPU        =    34.9758 [parent =    34.9758, child =    1.3e-05]
  Total wall clock =    247.892
```

Figure 2.10: PyNIC-DAKOTA system output file for determining the optimal parameters for ^{56}Mn in coal fly ash for NAA in the UUTR

```
<<<<< Function evaluation summary: 1000 total (1000 new, 0 duplicate)
<<<<< Best parameters          =
                      1.5711635142e-01 mass
                      2.3124152293e+00 IrrTime
                      4.4253775121e+01 DecayTime
                                 TI_10 irradPort
<<<<< Best objective function  =
                      8.4448263205e-06
<<<<< Best data captured at function evaluation 876


<<<<< Iterator soga completed.
<<<<< Environment execution completed.
DAKOTA execution time in seconds:
  Total CPU        =    34.5551 [parent =    34.5551, child =    1.7e-05]
  Total wall clock =    217.037
```

Figure 2.11: PyNIC-DAKOTA system output file for determining the optimal parameters for ^{139}Ba in coal fly ash for NAA in the UUTR

```
<<<<< Function evaluation summary: 1000 total (1000 new, 0 duplicate)
<<<<< Best parameters          =
                      2.8308207967e-01 mass
                      1.9058714858e+00 IrrTime
                      1.6980329685e+01 DecayTime
                                 TI_30 irradPort
<<<<< Best objective function  =
                      8.8075557609e-05
<<<<< Best data captured at function evaluation 932


<<<<< Iterator soga completed.
<<<<< Environment execution completed.
DAKOTA execution time in seconds:
  Total CPU        =    34.6261 [parent =    34.6261, child =    1.6e-05]
  Total wall clock =    247.522
```

Figure 2.12: PyNIC-DAKOTA system output file for determining the optimal parameters for ^{42}K in coal fly ash for NAA in the UUTR

Table 2.1: DAKOTA input variables

Variable Type	NAA Variable Description	Units and Values	
Continuous	Sample Mass	Grams	User Specified Range and Initial Point
	Irradiation Time	Minutes	
	Counting Delay Time	Minutes	
Discrete	UUTR Irradiation Port & Power Level (Refer to Fig. 1)	PI – 1 kW / 10 kW / 30 kW / 50 kW / 70 kW / 90 kW TI – 1 kW / 10 kW / 30 kW / 50 kW / 70 kW / 90 kW CI – 90 kW FNIF – 90 kW	

Table 2.2: PyNIC-DAKOTA system variable inputs for determining the optimal parameters for $^{59}Co \rightarrow ^{60}Co$ NAA in the UUTR

Variable Type	NAA Variable Description	Lower Bound	Upper Bound	Initial Point
Continuous	Sample Mass (g)	0.05	1.0	0.1
	Irradiation Time (min)	1.0	180.0	5.0
	Counting Delay Time (min)	5.0	1440.0	10.0
Discrete	UUTR Irradiation Port & Power Level	PI – 1 kW / 10 kW / 30 kW / 50 kW / 70 kW / 90 kW TI – 1 kW / 10 kW / 30 kW / 50 kW / 70 kW / 90 kW CI – 90 kW FNIF – 90 kW		

Table 2.3: PyNIC-DAKOTA system SOGA selected variables and PyNIC calculated objective function results for determining the optimal parameters for $^{59}Co \rightarrow ^{60}Co$ NAA in the UUTR

Iteration #	Sample Mass (g)	Irradiation Time (min)	Counting Delay Time (min)	Irradiation Port & Power Level (kW)	Obj_Fn
1	0.060	37.3	61.7	FNIF_90	21.283308
2	0.062	23.7	1152.2	PI_50	60.460221
3	0.073	123.2	166.1	TI_50	79.489973
4	0.079	157.9	229.8	PI_90	563.256422
5	0.093	39.0	569.6	PI_10	19.832471
6	0.096	42.4	780.0	PI_1	2.138914
7	0.100	77.6	89.3	CI_90	677.025249
8	0.106	122.0	1400.0	PI_70	435.215875
9	0.107	49.8	1357.2	TI_70	44.995168
10	0.123	150.2	1148.3	FNIF_90	85.862711
↓	↓	↓	↓	↓	↓
515	0.250	2.9	683.7	TI_1	0.017533241
516	0.259	1.5	53.7	TI_1	0.000606637
517	0.259	2.9	1413.1	TI_1	0.017526397
518	0.337	2.9	1220.1	TI_1	0.017528208
519	0.640	2.9	1374.5	TI_1	0.017526759
520	0.703	1.5	341.3	TI_1	0.000608031
521	0.703	1.5	1413.1	PI_10	0.745675418
522	0.703	2.9	1152.2	TI_10	0.355288454
523	0.887	2.9	1284.7	TI_1	0.017527601
524	0.963	1.5	708.0	TI_1	0.000609809
↓	↓	↓	↓	↓	↓
945	0.444	1.5	53.7	TI_1	0.0006066370263
946	0.521	160.2	21.6	TI_1	2.047941079
947	0.669	1.5	21.6	TI_1	0.0006064809978
948	0.706	1.5	21.6	TI_1	0.0006064809979
949	0.816	1.5	53.7	TI_1	0.0006066370263
950	0.444	1.5	21.6	TI_1	0.0006064809989
951	0.456	1.5	746.7	TI_1	0.0006099971251
952	0.483	1.5	21.6	FNIF_90	0.839252069
953	0.573	145.0	53.7	TI_1	1.851616162
954	0.598	107.4	21.6	TI_1	1.365728205
↓	↓	↓	↓	↓	↓
991	0.540	1.5	920.5	TI_1	0.0006108398229
992	0.593	1.5	21.6	TI_1	0.0006064809980
993	0.703	52.5	21.6	TI_1	0.656968633
994	0.752	81.4	21.6	TI_1	1.030174754
995	0.992	1.5	304.7	TI_1	0.0006078538665
996	0.456	1.5	21.6	PI_1	0.056594188
997	0.521	27.7	21.6	TI_1	0.336951777
998	0.554	96.5	21.6	TI_1	1.225388621
999	0.891	1.5	21.6	PI_70	5.341593126
1000	0.484	1.5	1182.3	TI_1	0.0006121089878

Table 2.4: Historical UUTR NAA data of the coal fly ash standard samples ^{56}Mn, ^{139}Ba and ^{42}K are only considered for testing PyNIC-DAKOTA system [32]

Sample #	Sample Mass (g)	Counting Delay Time (min)	Irradiation Port & Power Level (kW)	^{56}Mn activity (µCi/g)	^{139}Ba activity (µCi/g)	^{42}K activity (µCi/g)
1	0.161	8.5	TI_1	0.042	Not detected	Not detected
2	0.208	6.0	TI_1	0.036	Not detected	Not detected
3	0.189	11.0	TI_1	0.023	Not detected	Not detected
4	0.159	27.0	TI_10	0.350	0.037	Not detected
5	0.131	33.0	TI_10	0.350	0.046	Not detected
6	0.162	30.0	TI_10	0.320	0.037	Not detected
7	0.165	44.0	TI_30	1.050	0.110	0.083
8	0.118	53.0	TI_30	1.030	0.140	0.120
9	0.165	61.0	TI_30	1.020	0.120	0.150

Table 2.5: PyNIC-DAKOTA system variable inputs for coal fly ash to detect ^{56}Mn, ^{139}Ba, and ^{42}K

Variable Type	NAA Variable Description	Lower Bound	Upper Bound	Initial Point
Continuous	Sample Mass (g)	0.05	0.3	0.1
	Irradiation Time (min)	0.5	5.0	2.0
	Counting Delay Time (min)	5.0	65.0	10.0
Discrete	UUTR Irradiation Port & Power Level	PI – 1 kW / 10 kW / 30 kW / 50 kW / 70 kW / 90 kW TI – 1 kW / 10 kW / 30 kW / 50 kW / 70 kW / 90 kW CI – 90 kW FNIF – 90 kW		

Table 2.6: PyNIC-DAKOTA system SOGA-selected variables and PyNIC calculated objective functions for determining the optimal NAA Parameters for ^{56}Mn in coal fly ash in the UUTR

Iteration #	Sample Mass (g)	Irradiation Time (min)	Counting Delay Time (min)	Irradiation Port & Power Level (kW)	Obj_Fn
1	0.056	2.4	8.1	PI_10	1.747672
2	0.057	4.6	48.0	PI_10	2.853789
3	0.062	3.3	17.3	CI_90	41.561508
4	0.065	3.9	50.0	CI_90	42.754454
5	0.066	2.2	26.1	TI_90	2.761751
6	0.067	2.0	34.4	TI_90	2.439342
7	0.070	3.1	31.4	CI_90	37.185221
8	0.075	3.2	18.6	PI_90	15.924288
9	0.076	1.1	6.4	PI_30	2.373573
10	0.078	3.2	35.9	PI_1	0.172588
↓	↓	↓	↓	↓	↓
515	0.150	3.0	21.1	TI_1	0.015846193
516	0.176	1.3	21.1	TI_1	0.015437725
517	0.202	1.3	35.9	TI_1	0.017006659
518	0.202	1.3	21.1	TI_1	0.015414815
519	0.202	1.3	41.1	TI_1	0.017520085
520	0.202	2.2	41.1	TI_1	0.001991872
521	0.202	3.0	23.7	TI_1	0.015208009
522	0.202	3.0	41.1	TI_90	3.534479417
523	0.212	1.3	41.1	TI_1	0.017604997
524	0.212	1.3	41.1	TI_1	0.017520085
↓	↓	↓	↓	↓	↓
795	0.295	2.2	27.4	TI_1	0.0004177801408
796	0.296	2.1	30.5	TI_10	0.347823082
797	0.076	2.2	30.5	TI_1	0.0001443872217
798	0.125	2.2	30.5	TI_1	0.0001443872221
799	0.127	2.2	30.5	TI_1	0.0001443872221
800	0.179	2.5	35.9	TI_1	0.0036256274310
801	0.191	2.2	27.4	TI_1	0.0004177801408
802	0.202	2.2	38.2	TI_1	0.0014918244360
803	0.202	2.1	35.9	TI_1	0.0021354381950
804	0.202	2.1	49.0	TI_1	0.0042939005040
↓	↓	↓	↓	↓	↓
991	0.125	2.2	30.5	PI_30	4.423292715
992	0.134	2.2	30.5	TI_1	0.0001443872234
993	0.229	2.2	30.5	TI_1	0.0001510975484
994	0.078	2.2	30.5	PI_1	0.108801477
995	0.150	2.2	30.5	CI_90	26.26368706
996	0.247	2.2	10.3	TI_1	0.0036269946230
997	0.269	2.2	30.5	TI_10	0.358556128
998	0.288	2.2	30.5	TI_1	0.0001443872357
999	0.296	2.2	30.5	TI_1	0.0001510975484
1000	0.117	2.2	30.5	PI_50	7.400073846

Table 2.7: PyNIC-DAKOTA system SOGA-selected variables and PyNIC calculated objective functions for determining the optimal NAA Parameters for ^{139}Ba in coal fly ash in the UUTR

Iteration #	Sample Mass (g)	Irradiation Time (min)	Counting Delay Time (min)	Irradiation Port & Power Level (kW)	Obj_Fn
1	0.075	3.7	54.2	TI_10	0.011468519
2	0.082	2.1	7.2	TI_70	0.192786981
3	0.083	1.0	31.9	PI_90	0.286679822
4	0.085	2.8	44.3	PI_90	0.760615136
5	0.091	2.3	14.3	TI_1	0.021791728
6	0.093	4.7	55.0	FNIF_90	0.172867833
7	0.095	0.6	22.6	FNIF_90	0.006401042
8	0.101	2.2	21.2	PI_50	0.526181774
9	0.103	2.1	31.3	PI_1	0.015379175
10	0.104	2.7	57.8	PI_70	0.656314976
↓	↓	↓	↓	↓	↓
515	0.109	2.3	46.0	TI_10	0.000364993
516	0.192	2.1	46.0	TI_10	0.002491515
517	0.192	3.1	35.0	TI_10	0.010641459
518	0.200	2.3	45.4	TI_10	0.000256255
519	0.238	2.3	31.9	TI_10	0.002701373
520	0.238	2.3	45.4	TI_10	0.000256255
521	0.247	2.3	45.5	TI_10	0.000270135
522	0.276	2.3	46.0	TI_50	0.098175033
523	0.293	2.3	45.5	TI_10	0.000270135
524	0.060	2.1	46.0	TI_10	0.002491515
↓	↓	↓	↓	↓	↓
874	0.154	0.6	7.7	TI_30	0.0001266268
875	0.154	2.3	33.0	TI_10	0.0024478783
876	0.157	2.3	44.3	TI_10	0.0000084448
877	0.162	2.1	33.0	PI_90	0.6389407778
878	0.193	2.3	7.7	TI_30	0.0767403747
879	0.217	0.6	7.7	TI_10	0.0166244577
880	0.217	2.3	7.7	TI_30	0.0767403747
881	0.246	0.6	44.7	TI_10	0.0188490433
882	0.246	2.3	44.7	TI_30	0.0497176268
883	0.247	4.1	44.3	TI_10	0.0190943859
↓	↓	↓	↓	↓	↓
991	0.144	0.6	7.7	TI_30	0.0001266268
992	0.157	2.3	7.7	TI_10	0.0089134582
993	0.246	1.5	7.7	TI_30	0.0409088832
994	0.246	0.6	7.7	PI_50	0.1326619928
995	0.246	3.9	44.7	TI_10	0.0171741348
996	0.263	2.3	11.0	TI_10	0.0079932740
997	0.276	2.3	7.7	TI_30	0.0767403747
998	0.298	0.6	44.7	TI_30	0.0065471298
999	0.065	0.6	44.3	TI_30	0.0064836494
1000	0.088	0.6	44.3	TI_10	0.0189622184

Table 2.8: PyNIC-DAKOTA system SOGA-selected variables and PyNIC calculated objective functions for determining the optimal NAA Parameters for ^{42}K in coal fly ash in the UUTR

Iteration #	Sample Mass (g)	Irradiation Time (min)	Counting Delay Time (min)	Irradiation Port & Power Level (kW)	Obj_Fn
1	0.057	2.7	45.4	TI_70	0.419068538
2	0.061	4.6	23.4	PI_90	3.969424238
3	0.063	3.0	61.2	TI_10	0.095349919
4	0.065	4.8	29.1	PI_10	0.428798005
5	0.070	1.4	46.9	PI_70	1.086263104
6	0.072	2.4	64.6	PI_30	0.688798500
7	0.073	4.5	30.3	PI_10	0.392564659
8	0.073	2.2	38.3	PI_10	0.086637816
9	0.085	2.1	38.0	PI_50	1.145248741
10	0.092	1.9	9.0	TI_50	0.119926958
↓	↓	↓	↓	↓	↓
515	0.127	2.0	30.4	TI_30	0.011340255
516	0.192	1.8	30.4	TI_30	0.012440276
517	0.192	1.8	46.0	TI_30	0.015007661
518	0.192	2.0	30.4	TI_50	0.145567092
519	0.192	2.0	35.1	TI_30	0.010468741
520	0.236	1.8	17.2	TI_30	0.010225677
521	0.248	1.8	20.8	TI_70	0.228035805
522	0.248	1.8	29.5	TI_30	0.012283958
523	0.287	2.0	30.4	TI_30	0.011340255
524	0.296	1.8	30.4	TI_30	0.012440276
↓	↓	↓	↓	↓	↓
930	0.236	1.9	17.0	TI_30	0.00031459640
931	0.253	1.9	17.2	TI_30	0.00012124160
932	0.283	1.9	17.0	TI_30	0.00008807556
933	0.283	1.9	17.2	TI_30	0.00012124160
934	0.055	1.9	17.0	TI_30	0.00008807558
935	0.079	3.1	17.2	TI_30	0.12159649350
936	0.115	1.9	17.2	TI_30	0.00028136003
937	0.165	1.9	17.2	TI_30	0.00028327143
938	0.207	1.9	17.2	TI_30	0.00028136003
939	0.210	3.2	17.0	TI_30	0.13183004800
↓	↓	↓	↓	↓	↓
991	0.212	3.3	17.2	TI_30	0.13989230130
992	0.253	1.9	17.0	TI_1	0.18366960250
993	0.294	1.9	17.2	TI_30	0.00020486720
994	0.055	1.9	17.2	TI_30	0.00012124160
995	0.115	1.9	17.0	TI_30	0.00023809021
996	0.163	1.9	17.0	TI_30	0.00008807557
997	0.181	1.9	17.2	TI_30	0.00012124160
998	0.181	4.6	17.2	TI_30	0.26925632900
999	0.210	1.9	17.2	TI_30	0.00011933425
1000	0.212	1.9	17.2	TI_30	0.00020486720

Table 2.9: Optimal NAA parameters comparison for detecting ^{56}Mn, ^{139}Ba, and ^{42}K

		Optimal PyNIC-DAKOTA Parameters	UUTR Experimental Parameters
NAA for detecting ^{56}Mn at MDL	Sample Mass (g)	0.076	0.161-0.208
	Irradiation Time (min)	2.2	2.0
	Counting Delay Time (min)	30.5	8.5-11.0
	Irradiation Port & Power Level (kW)	TI – 1	TI – 1
NAA for detecting ^{139}Ba at MDL	Sample Mass (g)	0.157	0.131-0.162
	Irradiation Time (min)	2.3	2.0
	Counting Delay Time (min)	44.3	27.0-33.0
	Irradiation Port & Power Level (kW)	TI – 10	TI – 10
NAA for detecting ^{42}K at MDL	Sample Mass (g)	0.283	0.118-0.165
	Irradiation Time (min)	1.9	2.0
	Counting Delay Time (min)	17.0	44.0-61.0
	Irradiation Port & Power Level (kW)	TI – 30	TI – 30

CHAPTER 3

DACOS: DAKOTA-AGENT NEUTRONICS COMPUTATIONAL OPTIMIZATION SYSTEM[1]

3.1 Abstract

DACOS is a newly developed computational optimization system that merges well-known neutron transport code AGENT and well-known optimization tool DAKOTA. The DACOS can be applied to any reactor configuration for the purpose of optimizing its parameters such as but not limited to determining the optimal fuel composition and spatial distribution, amount and position of reflectors and neutron absorbing materials to achieve a specified neutron flux at a given location in the reactor or reactor power level. In this chapter, we provide detailed description of the DACOS system performances with the examples that include modeling of the University of Utah TRIGA research reactor to achieve a specific neutron flux in the center of the reactor by altering the fuel, reflectors, and neutron absorbing materials and their placement within the core. This research reactor DACOS model is also utilized in demonstrating its ability to determine the control rod placement and fuel placement to assure a desired k_{eff}. The DACOS demonstrated the ability to successfully optimize neutron flux and k_{eff}, and thus shows to be applied to any type and complexity of nuclear reactors.

---

[1] R. C. Schow, D. Kim and T. Jevremovic, "DACOS: DAKOTA-AGENT neutronics computational optimization system," *Ann. Nucl. Energy,* vol. 112, pp. 245-256, Feb. 2018.

3.2 Introduction

The design, modification and refueling of nuclear reactors results in many difficult optimization problems in nuclear engineering. There are competing factors for safety and efficient utilization of fuel during design, modification, and refueling. Nuclear fuel management optimization techniques of reactor core designs have been investigated for more than four decades [1]-[4]. Initially the nuclear reactor fuel optimization problem was solved manually by experts utilizing their knowledge and experience. Many of the historical studies have tried different optimization techniques such as linear and quadratic programming, dynamic programming, perturbation theory, and genetic algorithms [5]-[8].

Genetic algorithms have become a well proven and robust tool in the optimization of nuclear reactors due to their ability to not get trapped in local optima and give better results for global optimization [9]. The Design Analysis for Optimization and Terascale Applications (DAKOTA) is a flexible tool developed by Sandia National Labs that has the ability to implement a variety of genetic algorithms with simple interfaces [10]. DAKOTA's genetic algorithm optimization techniques can be utilized with a robust neutronics code system to generate a new tool for nuclear reactor core optimization.

The optimization and improvement of the neutronic analysis and configuration of nuclear reactors can result in the decrease of design margins, shortening of the development design cycle, a reduction of the lengthy testing programs in support of the design process, improving fuel consumption, neutron flux optimization, safety analysis, and improved operations [11]. The well-benchmarked and tested AGENT export-controlled computational neutronics code system is based on the R-functions solid modeler and the Method of Characteristics (MOC) [12]-[19]. AGENT can successfully provide detailed point-wise information about specific neutron flux and eigenvalues of any current or future fast or thermal spectrum power reactors or research and space reactor designs. Coupling the agile and powerful AGENT neutronics code system with the optimization toolkit from DAKOTA creates the DAKOTA-AGENT Computational Optimization System (DACOS).

The previous work on reactor core optimizations were constricted in their reactor applications. Many used highly specific programs that were designed specifically to determine core reloading patterns for specific cores or used simple neutronics codes that could only model basic core geometries. Many of the neutronics codes used in the optimization studies are outdated and limited in their diversification of capabilities. Using AGENT in the DACOS generates a new more capable reactor core optimization system than developed historically.

The majority of the activities, experiments and research that are conducted at research reactors require a specific neutron flux at a certain point in the reactor core or one of the experimental facilities. Paul et al. desired to activate and produce ^{54}Mn from ^{53}Mn in meteorites, which requires a high enough thermal neutron flux but a low fast neutron flux [20]. Meftah et al. and others have investigated maximizing the thermal neutron flux in a research reactor to produce radioisotopes [21], [22]. Historical investigations were interested in optimizing neutron fluxes and other parameters in research reactors and used various methods of calculations and codes to determine flux and then compare the calculations of one core configuration to another. In this chapter, we describe a novel approach to coupling a neutronics code system for a reactor core, AGENT, with Sandia National Laboratories optimization algorithm, DAKOTA, in thus successfully optimizing the research reactor core neutron flux using the DACOS [23].

3.3 Overview of the AGENT and DAKOTA methodologies

3.3.1 AGENT methodology

The Arbitrary GEometry Neutron Transport (AGENT) methodology is based on the R-function solid modeler approach, which allows basic modeling of complex geometries, joined with the method of characteristics (MOC) which solves the neutron transport equation along characteristic lines [24], [25]. The Boltzmann equation reduces to a total derivative along these characteristic lines. This methodology results in no limitations on geometry and allows for an accurate treatment of complex reactor systems [13]-[15]. This capability moves DACOS into a new area of optimization for reactor core assemblies.

The AGENT code system is well-documented and benchmarked on various reactor cores with a wide variety of geometries such as BWR, C5G7, TWOHEX, PUR-1, Modular High-Temperature Gas-Cooled Reactor (MHTGR), BN-600, VVER-1000, and the University of Utah TRIGA Reactor (UUTR) [12], [13], [16], [19], [26]. AGENT full scale models of the UUTR have been compared and benchmarked with MCNP6 models demonstrating high accuracy [19].

In order to model a steady-state reactor in 3-D, AGENT utilizes the 2-D/1-D coupled MOC equations through the neutron leakage term; general flow-chart of the AGENT methodology is depicted in Figure 3.1. In the AGENT methodology, the UUTR core is divided into 2-D radial planes, and therefore, a radial solution is obtained for each core plane configuration as seen on the left-hand side of Figure 3.1. A 1-D axial solution is then obtained for each pin region as shown on the left-hand side of Figure 3.1 [27]. Figure 3.1 displays the 2-D/1-D coupling iteration and convergence loop and also demonstrates the basic parameters of the MOC discretization used in the AGENT methodology.

The MOC equations in Figure 3.1 are solved as a fixed source problem with only the transverse leakage changing from one iteration to the next. A converged solution, in terms of angular flux and leakages, gives the computation a new eigenvalue. The fission source for both equations is then updated [13].

The flexibility of the R-function solid modeler and the accuracy and speed of the MOC results in AGENT being an excellent choice for a neutronics methodology to couple for optimization of any reactor design and geometry.

3.3.2 DAKOTA methodology

The DAKOTA (Design Analysis Kit for Optimization and Terascale Applications) project started in 1994 as an internal research and development activity at Sandia National Laboratories in Albuquerque, New Mexico [10]. One of the main focuses of DAKOTA was to provide engineers and scientists with a systematic and rapid means to obtain optimal designs or uncertainty or understand sensitivity using simulation-based models [28]. DAKOTA has a variety of iterative methods and meta-algorithms that can flexibly interface with different simulation codes. The principal classes of DAKOTA algorithms are the following: parameter studies, design of experiments, uncertainty quantification, optimization, and calibration. Sandia National

Laboratories has released the DAKOTA software as open source and is thus readily available for use and implementation.

DAKOTA has been utilized by many researchers and scientist in optimization and sensitivity analysis within the nuclear field. Recently, sensitivity analysis was performed utilizing DAKOTA coupled with a reactor severe accident core melt Matlab self-leveling model to determine the importance of model parameters for severe reactor accident debris bed properties [29]. DAKOTA's uncertainty analysis was also used to work with TRACE, thermal-hydraulic code, to analyze a postulated Large Break Loss of Coolant Accident (LBLOCA) in an AP1000 Pressurized Water Reactor (PWR) [30].

DAKOTA's optimization techniques have been demonstrated recently; DAKOTA was coupled with a neutronics code, NEWT, with DAKOTA's genetic search algorithm, Multi-Objective Genetic Algorithm (MOGA), to determine configurations of target fuels, spectral shift absorbers and positions of the target fuel pins for optimal transmutation performance in an AP1000 fuel assembly [31]. In this study, they varied the fuel types, fuel dimensions, spectral absorbers and fuel positions to determine the optimum transmutations of plutonium and minor actinides as a method to reduce the fuel stockpile without the use of fast reactors. In order to reduce computation time, the optimization was split into three stages and was successful in determining the optimal fuel and spectral absorber for the destruction of plutonium. This was a very specific use of coupling DAKOTA with NEWT for plutonium destruction.

The genetic algorithms, coliny_ea and SOGA, used in DAKOTA are based on Darwin's theory of survival of the fittest, which means the variables that give the most optimal outcome will continue to be copied and altered for future generations or solutions. Genetic algorithms start with an arbitrarily selected population of design points in the parameter space, where the values of the design variables form a “genetic string,” similar to DNA in a biological cell, that uniquely characterizes each objective function. The objective function is the calculation or result of the specific code, such as AGENT, that the genetic algorithm is trying to minimize [32].

Genetic algorithms have been used to develop fuel loading patterns for nuclear power reactors as well as the placement of burnable absorbers [33], [34]. The previous studies on the optimization of nuclear reactor cores generated individually tailored genetic algorithms designed for specific parameters [35], [36]. In this study, a generalized approach for research reactors neutronics code is coupled with a genetic algorithm optimization code that could be applied to any reactor or facility.

For the DACOS system, two optimization algorithms that minimizes an objective function were selected called, coliny_ea and SOGA. Both are genetic algorithms and are minimum optimization tools that apply the following generalized steps as depicted in Figure 3.2:

1. Chooses an initial population randomly and executes the function evaluations on these individuals.
2. Performs selection for parents based on relative fitness.
3. Applies crossover and mutation to generate new individuals from the selected parents.
4. Executes function evaluations on the new individuals.
5. Performs replacement to determine new population.
6. Returns to step 2 and continues the algorithm until convergence criteria is

satisfied or iteration limits are exceeded.

To illustrate the genetic algorithm method of obtaining solutions, an example of trying to generate a particular character string will be used. The targeted character string for this example is "AGENT." The method will include possible solutions that will be a string of fixed-length that is five characters long. The possible characters in a string will be one of the 26 valid characters (upper case letters "A" to "Z"). The objective function for the algorithm will be the summation of each character's point value and each character will receive one point for each position in the string that has the correct character. The correct answer has the possibility to have an objective function of 5 if it spells "AGENT."

Step 1 in the genetic algorithm is to randomly select an initial population and execute the objective function on each member of the population. The user can select the size of the population and for this example each population will be 10. Table 3.1 gives the initial population and their associated objective function value.

The initial population in Table 3.1 demonstrates that the candidate 5 has the best objective function of 2 with 2 characters out of the 5 that match the target string "AGENT." Step 2 selects the most fit parent candidates from the initial population which in this case candidates 1, 5, and 9 have objective function values > 0. Step 3 starts with the crossover of 2 parents. An example of crossover is given:

- Parent 1 (Candidate 1) – ASHTO
- Parent 2 (Candidate 5) – VNELT
- Offspring 1 – ASELT
- Offspring 2 – VNHTO

Crossover was implemented in this example after the second character. Offspring 1 now has an improved objective function of 3. This is how crossover leads towards a better solution. It is noted that if crossover was the only manipulation of the population, the best solution would not be achieved. One way to improve the likelihood of better results would be to increase the population size. Another method to improve results is including mutation in each iteration as well. Step 3 also includes mutation. Mutation is implemented by modifying each character in a string according to a given probability, such as 0.02 or 0.04. The probability would be that any single individual will be changed only slightly by mutation, or perhaps not at all. By applying mutation to each set of offspring produced in crossover, it allows for the possibility of new correct characters to be introduced. This process is reiterated many times until the algorithm converges on the desired solution of character strings.

3.4 The DAKOTA-AGENT Computational Optimization System (DACOS)

The flow chart of the DAKAOTA-AGENT Computational Optimization System (DACOS) is shown in Figure 3.3. The coupling process starts with a DACOS input file that begins the optimizer algorithm. This begins by DAKOTA generating an input parameters file that is then preprocessed to initiate AGENT. AGENT executes its calculations for neutron flux and/or k_{eff} and is postprocessed into a file for the DAKOTA optimizer to utilize in the optimization calculations. This process is then repeated until an optimal solution is obtained.

The DAKOTA input file contains six different blocks labeled: *environment, method, model, variables, interface, and responses*:

- *Environment block*: gives the overall DAKOTA settings such as tabular and graphical data output settings (block is optional).
- *Method block*: the user identifies the iterative method such as optimization, uncertainty quantification, calibration, or parameter studies DAKOTA will employ and that method's associated options.
- *Model block*: optional block that provides the analytical unit for controlling how a set of variables is mapped through an interface into a set of responses when needed by an iterative method.
- *Variables block*: selects the number, type, and characteristics of the parameters that will be varied.
- *Interface block*: maps the variables into responses as well as specifics on how DAKOTA will pass data to and from the coupled code like AGENT.
- *Responses block*: specifies the types of data that the interface will return to DAKOTA.

The critical blocks for the coupling of AGENT to DAKOTA are the *method, variables, and interface* blocks; the execution and variables that AGENT is expecting are specified in these blocks and are further explained:

- *Method block*: the coliny_ea or SOGA iterative method is specified. The iterative method options such as the maximum iterations or convergence criteria, crossover type, and mutation type are selected. The population size for each generation can also be specified in this block.
- *Variables block*: the variables are split into continuous and discrete variables. AGENT requires discrete variables in the DACOS. Discrete variables may involve

a set of integer values (e.g., core material can be 1, 7, or 10), a range of consecutive integers (e.g., core material can be any integer between 1 and 11), a set of string values (e.g., core material can be "water," "fuel," or "reflector"), or a set of real values (e.g., core material can be identically 2.1, 5.2, or 6.8). The discrete variables that are changed in the DACOS are the materials in specified cells of the reactor that is modeled in the core as seen in Figure 3.4 and Table 3.2. DAKOTA adjusts the variables in order to locate an optimal design for a desired neutron flux or k_{eff}. DAKOTA interfaces with other simulation codes, like AGENT, by communicating through the file system. This is accomplished through the reading and writing of parameters and results files labeled "DAKOTA Input Parameters" and "DAKOTA Optimization Parameters" as seen in Figure 3.3. An example "DAKOTA Input Parameters" file is given in Figure 3.5.

- *Interface block*: DAKOTA calls AGENT into execution. A pre- and post-processing environment was needed to convert the "DAKOTA Input Parameters" file (Figure 3.5) and the "DAKOTA Optimization Parameters" file into the formats AGENT and DAKOTA are expecting, respectively.

AGENT then executes its methodology and determines the neutron flux for a specified location or k_{eff} of the core. The intended goal for the DACOS is to achieve a specified k_{eff} of the core or neutron flux at a specific location. In order for DAKOTA to determine the input parameters (cell materials) needed to achieve the target k_{eff} or flux, the calculated k_{eff} or flux from AGENT is inserted into an objective function. The optional objective functions (Obj. Fn) are given:

$$\text{Obj. Fn} = |calculated\ neutron\ flux - targeted\ neutron\ flux| \tag{3.1}$$

$$\text{Obj. Fn} = \left|calculated\ k_{eff} - targeted\ k_{eff}\right| \tag{3.2}$$

The objective function is needed to optimize a value near the targeted neutron flux or k_{eff} and is the output that the genetic algorithm is minimizing. DAKOTA iterates until a convergence criteria specified by the user is met. Once this is complete, an output file is generated providing the best combination of core materials to achieve the targeted value.

3.5 DACOS benchmark examples

The University of Utah TRIGA Reactor (UUTR) is a standard design nominal 100 kW_{th} MARK-I natural-convection-cooled pool reactor and is licensed by the U.S. Nuclear Regulatory Commission (NRC). The UUTR uses solid fuel elements, developed by General Atomics (GA), in which the zirconium-hydride moderator is homogeneously combined with enriched uranium. The reactor core consists of 127 cylindrical channels or cells for fuel elements, reflectors, moderator, experimental facilities, and control rods, which are contained between top and bottom aluminum grid plates. The top grid plate is arranged with 6 concentric rings around a central port as seen in Figure 3.4. The UUTR contains a lattice of 78 cylindrical stainless-steel-cladding uranium-zirconium hydride ($U\text{-}ZrH_{1.6}$) fuel-moderator elements (SS) and aluminum-cladding uranium-zirconium hydride ($U\text{-}ZrH_{1.0}$) fuel-moderator elements with three control rods located in the D-ring. The control rods are each controlled by their own driver and are called the safety, shim and regulating rods. The control rods are made of aluminum clad boron carbide and are not all the same size. Neutron reflection is provided in the radial direction by 12 graphite and 12 heavy water elements in an aluminum cladding. The UUTR is utilized for a variety of experiments, research, education, and training which most often use the four irradiation facilities: Central Irradiator (CI) located in the A1 cell, Pneumatic Irradiator (PI) located in the D4 cell, Fast Neutron Irradiation Facility (FNIF) located immediately outside the core with no reflectors in between, and Thermal Irradiator (TI) located immediately outside the core with graphite reflectors in between and filled with heavy water.

Experiments, research and tests being conducted at the UUTR could be enhanced and performance improved by targeting and achieving certain UUTR parameters, such as neutron flux, in specific areas of the core and experimental ports. This is accomplished by the DACOS providing the UUTR operators and staff with a guide to rearrangement of the UUTR core materials to obtain desired core parameters. For the DACOS UUTR benchmark examples, DAKOTA varies the UUTR cell materials with the given values as seen in Table 3.2, to achieve a targeted neutron flux value or k_{eff}.

In this example, the AGENT simulation parameters are given in Table 3.3. The azimuthal angles are spaced uniformly in the 2D plane from 0 to 2π [37]. For the UUTR benchmark using 24 azimuthal angles results in an azimuthal weight of 1/24. Leonard and McDaniel's two polar angles distribution (59.96˚ and 15.88˚) and their corresponding weights (0.860527 and 0.139473) provide accurate results for a given core complexity [38]. The ray separation is the uniform distance between each ray. The boundary of each cell is divided into boundary edges that accumulate neutron angular flux values per landed ray and then average the value over the number of arrivals; the average neutron angular flux value is used for each new ray starting from that boundary edge along the reflected direction [19]. The 44 boundary edges per core face were selected to ensure that when the cells where combined to form the full core model, the boundary edges align for the flux to be transferred to the adjacent assembly. The geometry sub-meshing divides the material zones into smaller areas that are assumed to have constant flux and source values.

3.5.1 Achieving required k_{eff} while changing the material in the central cell of the UUTR

The initial benchmark of the DACOS varies the central cell (A1) material in the full 3-D model of the AGENT UUTR to obtain a desired k_{eff}. The AGENT input file expects a numerical value (1-11) for each cell position of the UUTR as seen in Figure 3.4. In this benchmark, the central position, A1, is the only discrete variable that DAKOTA is altering with the 11 different materials listed in Table 3.2. Hence, this simple benchmark only has 11 different iterations and solutions. All three control rods in cells D4, D7, and D13 of the UUTR were fully inserted into the core for this benchmark. Table 3.4 gives the varied cell materials and the resulting k_{eff} calculated by AGENT and written back to DAKOTA.

Before running the DACOS benchmark, the k_{eff} of the UUTR with the central cell selected as a stainless steel-clad fuel rod was determined by running AGENT. The k_{eff} was determined to be 0.98249. This value was used as the desired k_{eff} for this DACOS benchmark. The DACOS found the trivial solution in the first iteration but still evaluated all 11 possibilities to ensure the optimal solution was found. Eq. (3.2) was utilized as the objective function in this benchmark.

The results also match the expected values of k_{eff} given the k_{eff} in iteration #8 with water selected as the center cell material matches the actual material used during UUTR operations and was determined to be 0.97606±0.00004 using MCNP6, [18]. DACOS determined the normal k_{eff} to be 0.97664. The highest k_{eff} values were found when fuel elements were placed in the A1 cell (DAKOTA Iterations 1, 2, and 8) while the lowest k_{eff} values were obtained when a control rod was selected (DAKOTA Iterations 3, 4, and 5). The safety and shim control rods are made of the same materials and are the same size which means when the two control rods were selected as the central cell materials it would be expected that they would produce the same k_{eff} and this was demonstrated as seen in iterations 3 and 4.

3.5.2 Comparison of DACOS algorithms by targeting neutron flux in 2D AGENT model of the UUTR

The center cell of the UUTR, A1, is also the Central Irradiator (CI), see Figure 3.4, and the location of the highest neutron flux irradiation facility in the UUTR is approximately 7.4×10^{12} n/(cm^{2}s) at 90 kW$_{th}$. The DACOS was used to determine a targeted total neutron flux value in the CI from altering the B2, B4, and B6 cell materials. In order to reduce computational redundancy, the only materials selectable to alter by DAKOTA in this comparison are given in Table 3.5. Some of the materials in Table 3.2 are very similar so materials with similar properties were eliminated.

A comparison of the coliny_ea and SOGA genetic algorithms in the AGENT-

DAKOTA system is given with a population size of 20 selected to conduct the example. Eq. (3.1) is the objective function used with a targeted total neutron scalar flux of 4.341×10^{-2} in the CI. This neutron scalar flux value was chosen as the target because it is approximately the same as the total neutron scalar flux in the CI when AGENT was run with only stainless steel-clad fuel in the B-Ring. This allows a test of the two different algorithms to see if they will find the expected solution of stainless steel fuel for all cells. The coliny_ea and SOGA results are given in Table 3.6. The coliny_ea method completed 136 iterations before converging and the SOGA method completed 87 iterations before converging.

The best solution that coliny_ea determined is in iteration #74 with materials as seen in Figure 3.6(a) of two stainless steel-clad fuel with one aluminum-clad fuel which gives an Objective Function of 2.23×10^{-3} while the SOGA optimal solution is found in iteration #49 with materials as displayed in Figure 3.6(b) of three stainless steel-clad fuel elements which gives an Objective Function of 6.5×10^{-4}. The results from this comparison show that SOGA found the more optimal solution within a shorter number of iterations as compared to the coliny_ea algorithm.

3.5.3 Obtaining neutron flux in the central irradiator by changing the B-Ring cell materials in 3D AGENT model of the UUTR

A full three-dimensional (3D) AGENT model of the UUTR is used in this benchmark of the DACOS. The target of this benchmark is to achieve a specific value of total neutron scalar flux in the CI of 1.224×10^{-5}. This is approximately the value determined from a previous run of the AGENT code with all B-Ring materials being selected as stainless-steel fuel elements. This was done to see if DACOS is working correctly. The DACOS targets a specific neutron flux in the center of the core by altering the B2, B4, and B6 cells as can be seen in Figure 3.4. The discrete variable materials selectable by the DACOS is given in Table 3.5. The Objective Function that the SOGA method will be implementing is Eq. (3.1). The SOGA was chosen over coliny_ea to complete the larger 3D model runs because it was found to converge quickly on the correct solution in the 2D comparison benchmark.

The DACOS implemented 47 iterations and assembled 26 population sets of 10 as seen in Table 3.7. The optimum solution was found in iteration #29 of all stainless steel-clad fuel elements in B2, B4, and B6 cells. The DACOS found the correct solution of all stainless steel-clad fuel elements.

A mid-plane view of the thermal energy neutron scalar flux (10^{-6} ~ 0.125 eV) from Iteration #29 is plotted in Figure 3.7 and from Iteration #18 in Figure 3.8. Figure 3.7 shows the normalized scalar flux distribution for the UUTR core with stainless steel fuel rods in cells 1-3 whereas Figure 3.8 shows the normalized scalar flux distribution for the core with graphite, water, and a control rod in cells 1, 2, and 3, respectively. The differences as seen between Figures 3.7 and 3.8 are indicated with a circle in the center where the normalized scalar flux is ~0.0014 and constant around the center position that is approximately 0.003 as can be seen in Figure 3.7 but three distinct circles are indicated around the center position in Figure 3.8. The stable normalized scalar flux values around the center of the core with all stainless-steel fuel rods (Figure 3.7) are consistent with what is expected during normal operations. The small circle above the center position that has normalized scalar flux values of ~0.00002 near the center of Figure 3.8 is the control rod, the small circle with normalized scalar flux values of ~0.0025 is the water and the small circle with normalized scalar flux values of ~0.0029 is the graphite reflector. The lower normalized scalar flux values from the location of the inserted control rod and the higher normalized scalar flux values from the inserted graphite and water in Figure 3.8 are also expected.

3.5.4 Targeting k_{eff} by changing the position of a control rod in the UUTR benchmark of DACOS

A relationship has been established between the reactivity insertion and the reactor power at the UUTR [39]. Utilizing the established relationship between reactor power and reactivity insertion, the DACOS could be used to determine the correct rod positions for a desired power level or to determine the maximum power obtainable by the current core configuration. This is accomplished by DAKOTA altering the rod position and AGENT computing the k_{eff} associated with the various rod positions.

The UUTR has three control rods, which are used to control reactor operations. The “safety” control rod has the highest worth and has an experimentally determined reactivity worth of \$2.233±0.179, next is the “shim” control rod with an experimentally determined reactivity worth of \$1.507±0.092 and the lowest worth rod is the “regulating” control rod with a worth of \$0.276±0.009 [40]. During normal operations of the UUTR, the “safety” control rod is fully withdrawn (100%), the “regulating” control rod is withdrawn partially out of the core at 65% withdrawn, and the “shim” control rod is varied in its position to control reactor power in a range of usually 50% – 78% withdrawn which corresponds to 1 kW – 90 kW.

The DACOS is set up in this example with the “safety” control rod fully withdrawn, 100%, and the “regulating” rod withdrawn to 65% while DAKOTA alters the withdrawn position of the “shim” rod in 6.66% increments. Both the coliny_ea and SOGA algorithm methods were tested for control rod positioning. A target k_{eff} of 1.000 was input into the DACOS for it to alter the “shim” rod and find the percent withdrawn position closest to this value, which corresponds to approximately 5.5 kW of power [39].

The results as seen in Table 3.8 match closely with similar “shim” withdrawn percentages from [39] such as a “shim” withdrawn of 60.1% had a MCNP5 k_{eff} value of 1.00139 which matches closely with the DACOS result of 1.00170 for 60.0%. Cross planes of the normalized thermal energy neutron scalar flux (10^{-6} ~ 0.125 eV) from Iteration #5 and #12 are plotted in Figures 3.9 and 3.10, respectively. The vertical planes in the figures that are circled show the difference from when the shim control rod is partially inserted (Figure 3.9) versus when it is fully withdrawn (Figure 3.10). The lower normalized scalar flux value channels of ~0.00002 can be seen in the vertical plane that are circled in Figure 3.9 when the control rod is partially inserted and the normalized scalar flux values of 0.0018-0.0025 are circled in the vertical plane in Figure 3.10 when water is present instead of the control rod due to its withdrawal. These results demonstrate the ability for DACOS to find optimal rod positions for obtaining various power levels.

3.6 Conclusion

A new neutronic optimization system was developed by coupling the neutronics code system, AGENT, with the flexible optimization software, DAKOTA, to form the

DAKOTA-AGENT Computational Optimization System (DACOS). The DACOS can be applied to any nuclear reactor design for optimizing the desired parameters such as but not limited to reactor fuel distribution and enrichment, power level, control rod positions. DAKOTA's optimization algorithms are robust and integrate well with AGENT. Two genetic algorithms from DAKOTA's library, SOGA and coliny_ea, were implemented and compared within the DACOS for a few representative benchmark examples. The benchmark examples were developed for the University of Utah TRIGA Reactor (UUTR). The DACOS was tested for the arrangement of core materials in order to obtain k_{eff}, specific neutron flux and/or reactor power values. The DACOS was also used to change the amount of rod withdrawal in the UUTR to obtain a given k_{eff}. Results from the DACOS benchmarks were compared to MCNP calculations of the UUTR in showing expected agreement. The future use of DACOS is targeted toward optimizing a neutron activation or material irradiation experiments given the UUTR has four different ports available for sample irradiations; equally DACOS can be applied to redesigning the UUTR core in raising its licensed power should that be desired. The DACOS is flexible in that it can be used for any type of a reactor of any level of complexity including also the large power reactors.

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3.8 References

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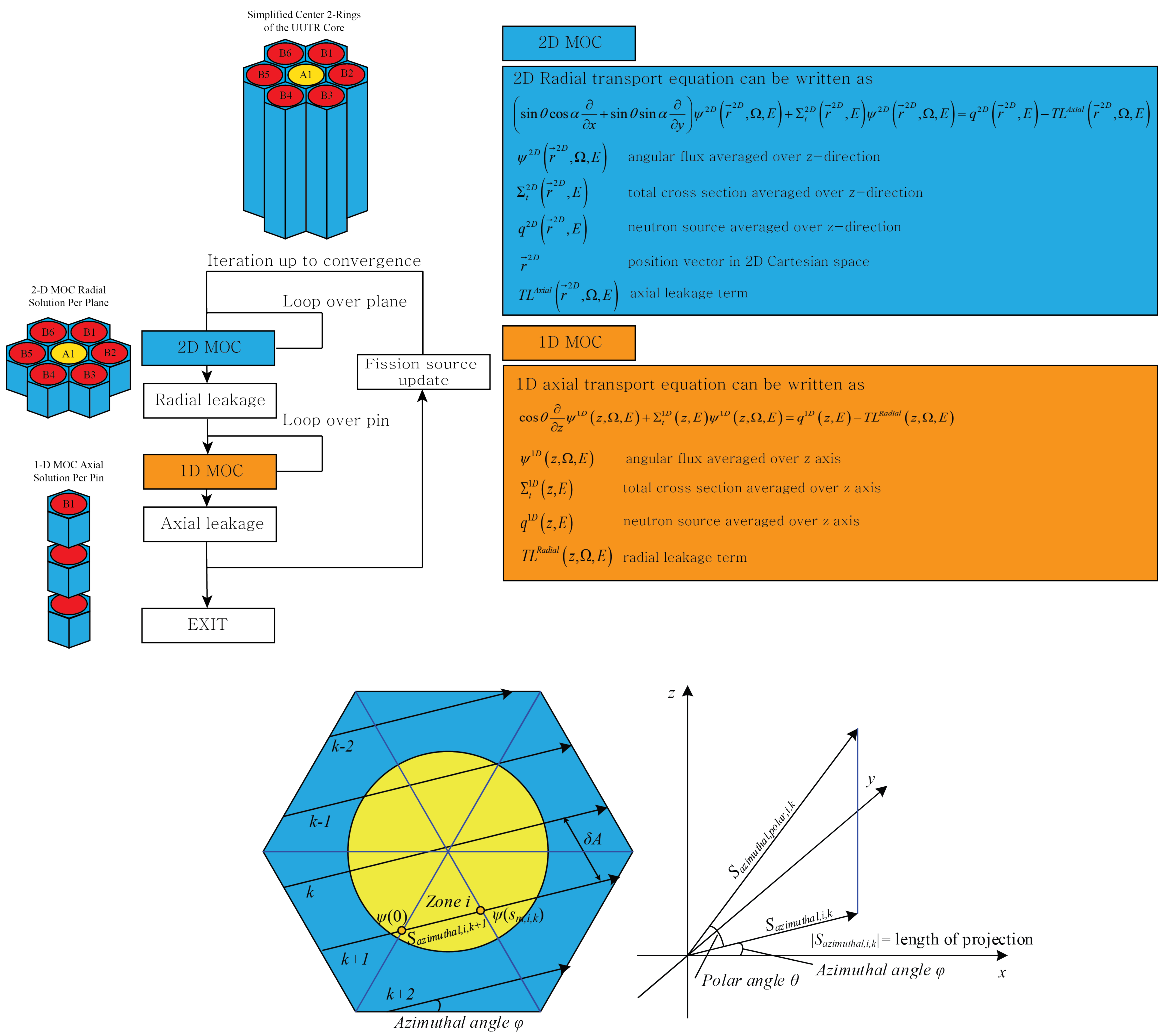


Figure 3.1: 2-D/1-D AGENT coupling solution for evaluation of the UUTR geometry

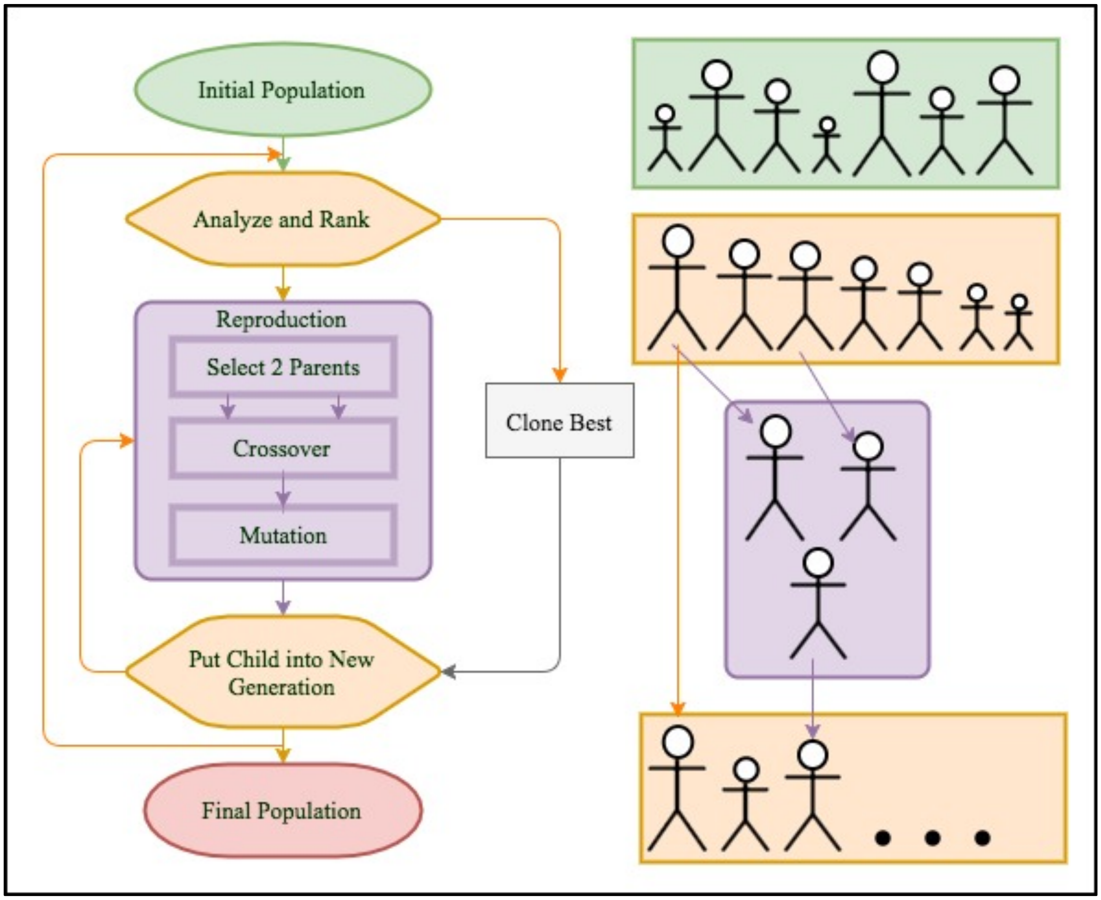


Figure 3.2: DAKOTA genetic algorithm methodology

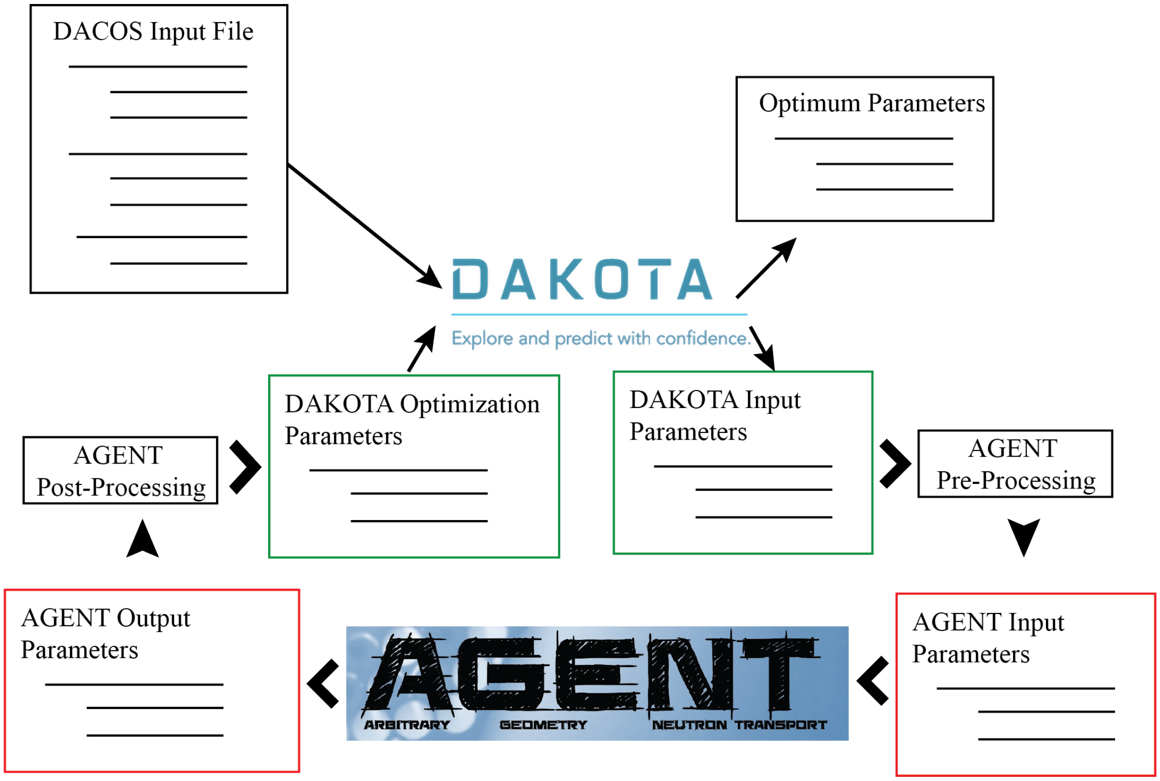


Figure 3.3: Flow chart of the DAKOTA-AGENT optimization system (DACOS)

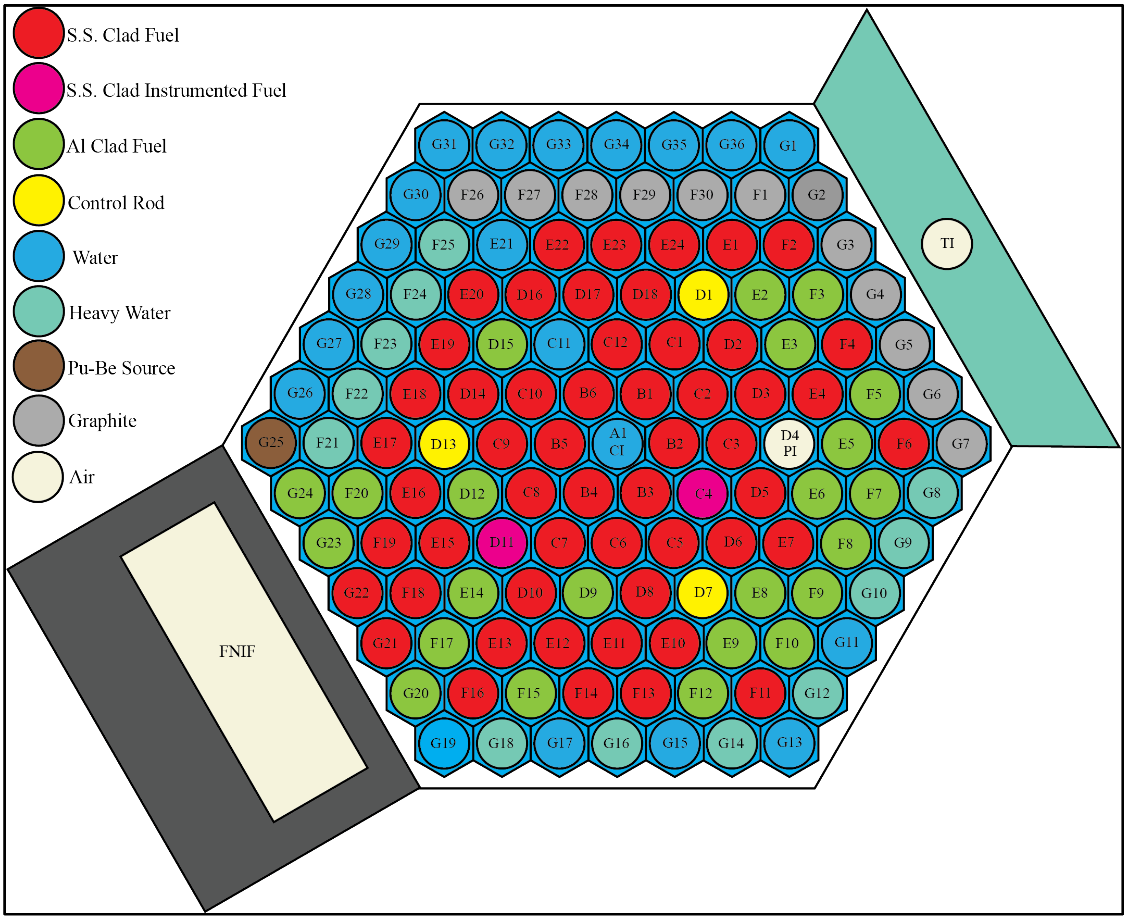


Figure 3.4: UUTR core configuration and irradiation facilities – total neutron flux ranges from highest in CI=7.4x10^{12} n/(cm^{2}s) to lowest in TI=7.3x10^{11} n/(cm^{2}s)

```
{ DAKOTA_VARS     =                    3 }
{ cell1           =                    1 }
{ cell2           =                    1 }
{ cell3           =                    7 }
{ DAKOTA_FNS      =                    1 }
{ ASV_1:CI_flux   =                    1 }
{ DAKOTA_DER_VARS =                    0 }
{ DAKOTA_AN_COMPS =                    0 }
{ DAKOTA_EVAL_ID  =                    1 }
```

Figure 3.5: Example DAKOTA Input Parameters file – 3 discrete variables (cell1, cell2 and cell3) are given discrete values of 1, 1, and 7 and the function that is being optimized is the CI_flux

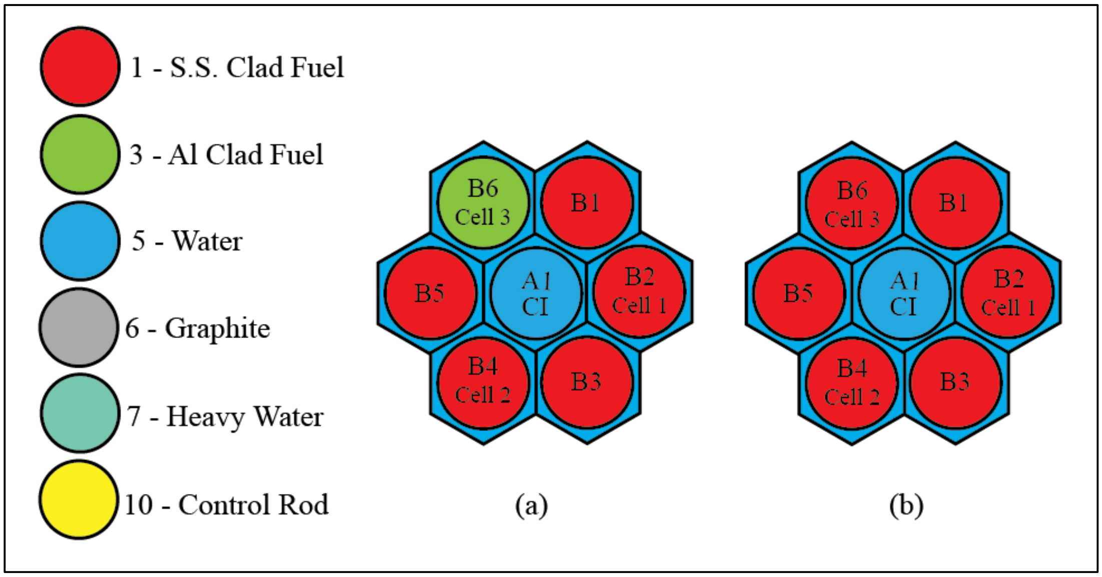


Figure 3.6: DACOS Solutions (a) coliny_ea and (b) SOGA for target flux in CI by altering B-Ring materials

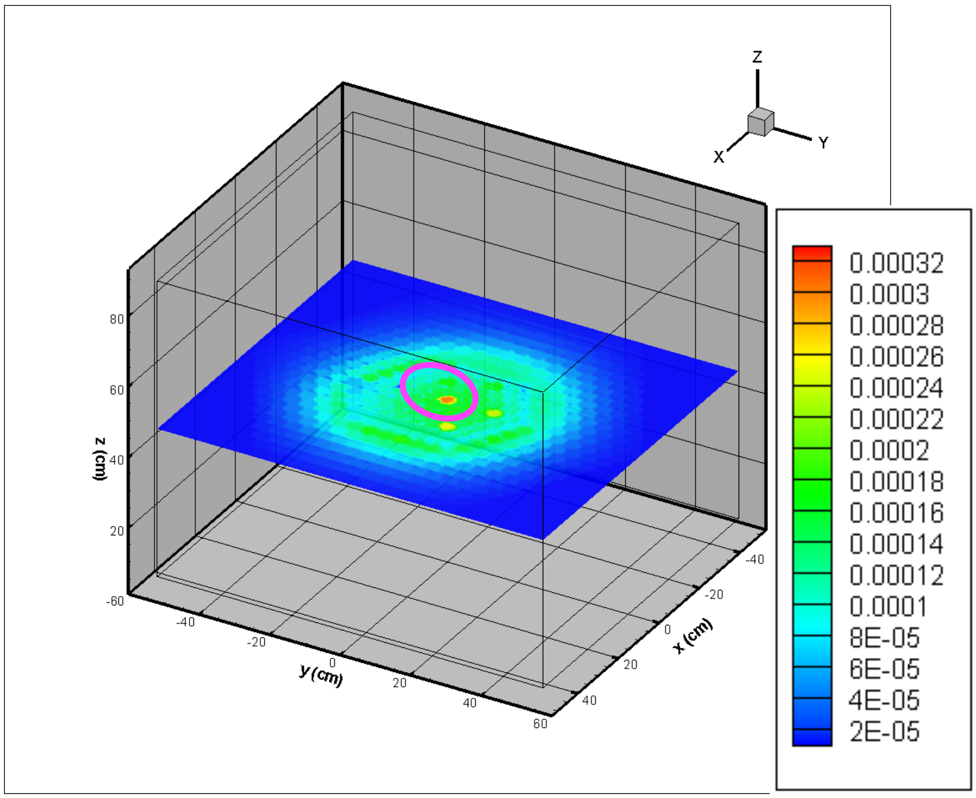


Figure 3.7: Normalized thermal scalar flux mid-plane view of iteration #29 in the DACOS 3D UUTR model

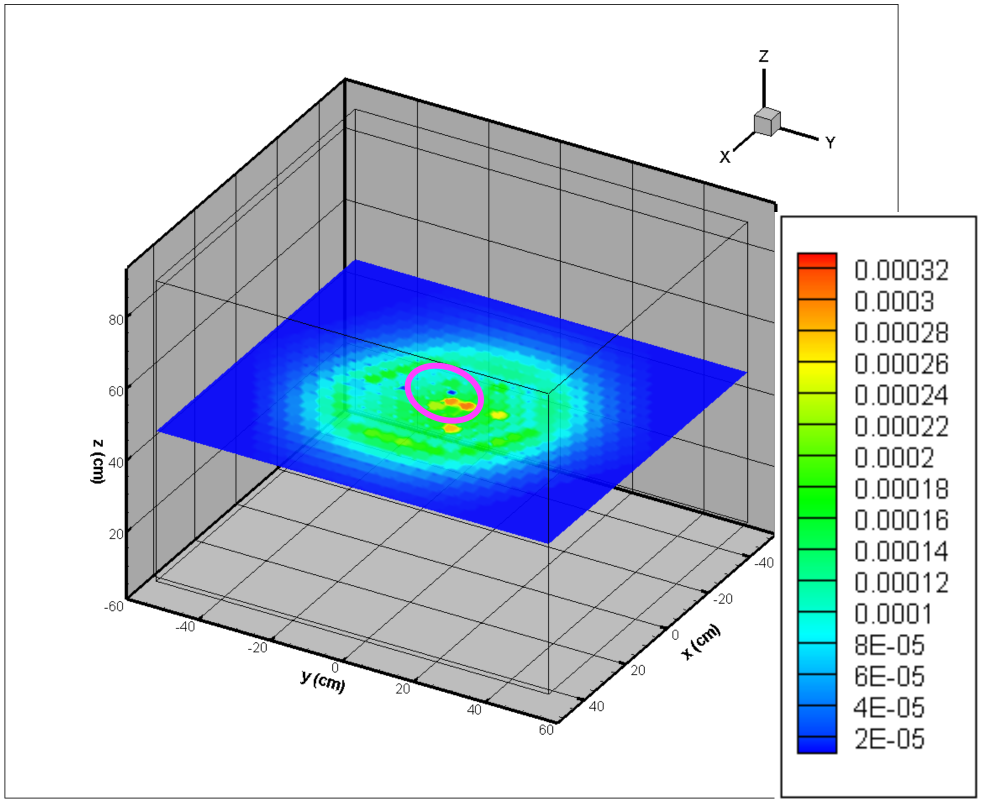


Figure 3.8: Normalized thermal scalar flux mid-plane view of iteration #18 in the DACOS 3D UUTR model

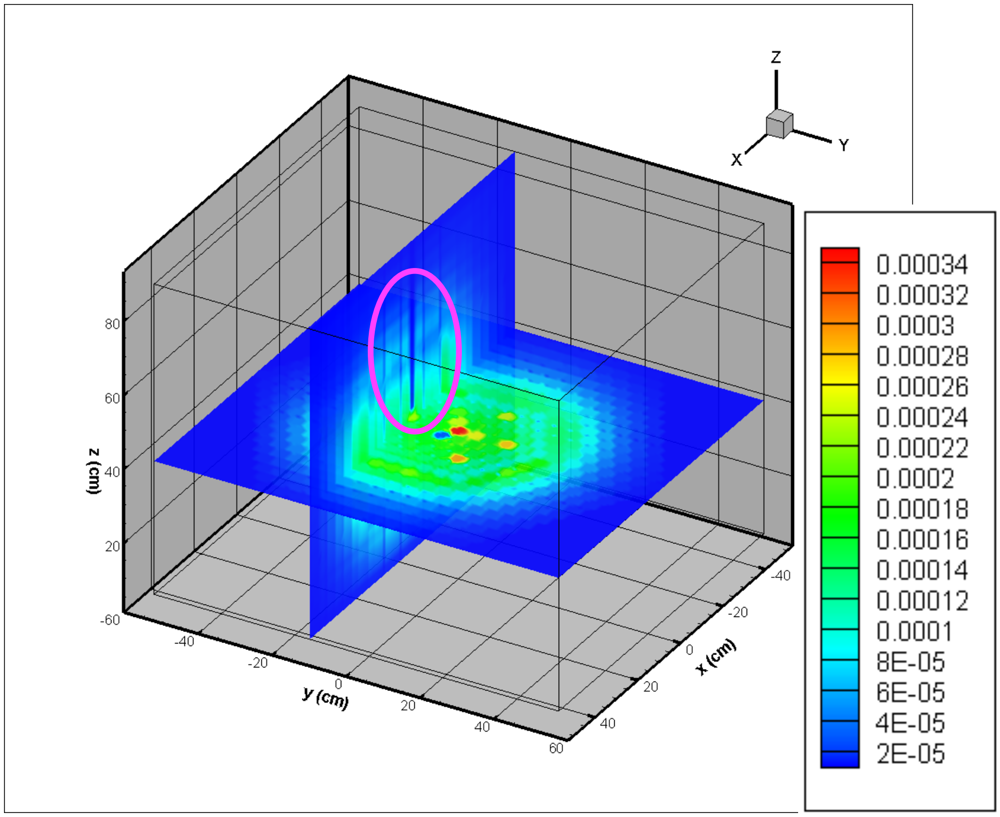


Figure 3.9: Normalized thermal scalar flux cross-plane views of iteration #5 in the DACOS 3D UUTR model

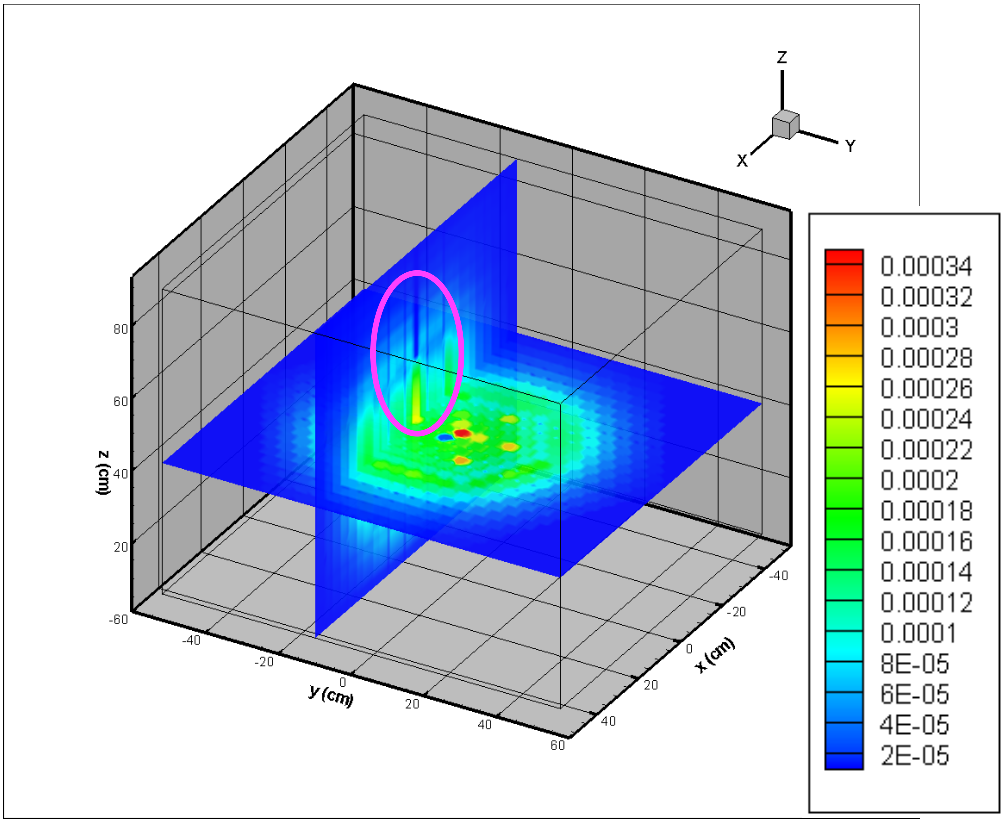


Figure 3.10: Normalized thermal scalar flux cross-plane views of iteration #12 in the DACOS 3D UUTR model

Table 3.1: Coliny_ea algorithm example: generate "AGENT" character string

	Initial Population	
Candidate	Character Strings	Objective Function
1.	ASHTO	1
2.	VKWVD	0
3.	FIUEI	0
4.	JKDIQ	0
5.	VNELT	2
6.	OAFRP	0
7.	CWAJP	0
8.	HVYJF	0
9.	JWEAK	1
10.	VRTHJ	0

Table 3.2: DAKOTA input variables

Variable Type	Variable Description	Values
Discrete	Cell Material	1 – Stainless Steel-Clad Fuel
		2 – Stainless Steel-Clad Instrumented Fuel
		3 – Aluminum-Clad Fuel
		4 – Reflector
		5 – Water Rod
		6 – Graphite
		7 – Heavy Water
		8 – Water
		9 – Regulating Control Rod
		10 – Safety Control Rod
		11 – Shim Control Rod

Table 3.3: AGENT simulation parameters for the DACOS UUTR benchmarks

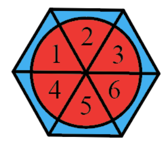
Parameter	AGENT
Number of Azimuthal Angles	24
Number of Polar Angles and Scheme	2, Leonard-McDaniel
Ray Separation (cm)	0.05
Number of Boundary Edges per Core Face	44
Geometry Sub-meshing	6 Triangles per Hexagonal cell assembly 
AGENT converging criteria for flux and eigenvalue	10^{-6}

Table 3.4: DACOS benchmark - A1 cell material DAKOTA iterations, the AGENT determined k_{eff} and the DACOS resulting objective function (Obj. Fn)

Iteration of DAKOTA	Central Cell (CI or A1) Material	k_{eff}	Obj. Fn
1	1 – Stainless Steel-Clad Fuel	0.98249	0
2	2 – Stainless Steel-Clad Instrumented Fuel	0.98206	0.00043
3	10 – Safety Control Rod	0.96285	0.01964
4	11 – Shim Control Rod	0.96285	0.01964
5	9 – Regulating Control Rod	0.97355	0.00894
6	8 – Water	0.97664	0.00585
7	4 – Reflector	0.97644	0.00605
8	3 – Aluminium Clad Fuel	0.98265	0.00016
9	5 – Water Rod	0.97669	0.00580
10	7 – Heavy Water	0.97501	0.00748
11	6 – Graphite	0.97732	0.00517

Table 3.5: DAKOTA input variables for targeting neutron flux by changing B-ring materials

Variable Type	Variable Description	Values
Discrete	Cell Material	1 – Stainless Steel-Clad Fuel
		3 – Aluminum-Clad Fuel
		5 – Water Rod
		6 – Graphite
		7 – Heavy Water
		10 – Safety Control Rod

Table 3.6: DACOS results targeting neutron scalar flux of 4.314x10^{-2} in 2D AGENT UUTR CI by altering B-ring materials

coliny_ea Results

Iteration #	Cell 1 (B2)	Cell 2 (B4)	Cell 3 (B6)	Obj. Fn
1	5	5	5	0.01845
2	5	10	10	0.02007
3	10	6	3	0.01667
4	10	10	10	0.02092
5	3	10	5	0.01474
6	10	1	3	0.00983
7	5	7	1	0.00947
8	1	3	6	0.00831
9	10	7	5	0.01576
10	6	3	1	0.00956
↓	↓	↓	↓	↓
71	6	1	5	0.01265
72	3	3	5	0.00969
73	5	1	10	0.01326
74	1	1	3	0.00223
75	1	3	3	0.00417
76	10	6	6	0.02040
77	7	3	10	0.01219
78	1	6	3	0.00887
79	7	10	10	0.01712
80	5	3	6	0.01491
↓	↓	↓	↓	↓
127	10	5	7	0.01664
128	10	7	7	0.01316
129	1	10	6	0.01326
130	5	6	10	0.01975
131	1	7	6	0.00892
132	10	6	1	0.01511
133	3	10	7	0.01197
134	3	10	1	0.00987
135	6	10	5	0.01969
136	1	10	10	0.01362

SOGA Results

Iteration #	Cell 1 (B2)	Cell 2 (B4)	Cell 3 (B6)	Obj. Fn
1	1	1	7	0.00289
2	1	1	10	0.00692
3	1	5	7	0.00898
4	1	10	10	0.01362
5	3	1	5	0.00772
6	3	7	6	0.01070
7	3	7	10	0.01117
8	3	10	1	0.00987
9	5	1	6	0.01289
10	5	3	1	0.00914
↓	↓	↓	↓	↓
41	7	1	1	0.00418
42	7	1	10	0.01045
43	7	5	7	0.01287
44	10	7	6	0.01624
45	1	5	1	0.00674
46	3	5	7	0.01088
47	7	7	1	0.00704
48	10	1	7	0.01036
49	1	1	1	0.00065
50	1	3	5	0.00772
↓	↓	↓	↓	↓
78	3	7	3	0.00641
79	7	5	3	0.01174
80	3	3	6	0.01029
81	7	3	3	0.00750
82	1	10	7	0.01009
83	6	1	3	0.00906
84	7	3	5	0.01122
85	10	7	1	0.01054
86	6	3	1	0.00956
87	10	1	1	0.00820

Table 3.7: DACOS results targeting neutron scalar flux of 1.224×10^{-5} in 3D AGENT UUTR CI by altering B-ring materials

Iteration #	Cell 1 (B2)	Cell 2 (B4)	Cell 3 (B6)	Obj. Fn
1	1	3	3	1.324E-07
2	3	1	7	3.719E-07
3	3	6	6	4.063E-08
4	5	3	6	1.161E-07
5	5	3	7	5.419E-07
6	5	10	1	6.375E-07
7	6	6	10	4.352E-07
8	7	1	5	6.371E-07
9	7	5	6	6.809E-07
10	7	10	7	1.380E-06
11	3	5	6	1.440E-07
12	3	10	1	4.197E-07
13	5	1	1	1.681E-07
14	7	1	6	4.924E-07
15	7	3	7	8.183E-07
16	1	1	6	6.517E-09
17	6	3	7	3.419E-07
18	6	5	10	6.126E-07
19	6	6	6	1.745E-08
20	7	3	3	3.451E-07
21	1	1	7	3.746E-05
22	3	3	3	1.999E-07
23	3	3	7	3.055E-07
24	5	1	6	1.837E-07
25	6	3	6	9.158E-08
26	3	1	6	6.096E-08
27	3	3	6	1.292E-07
28	5	5	6	3.960E-07
29	1	1	1	5.366E-11
30	6	5	6	1.910E-07
31	6	3	3	1.707E-07
32	1	6	6	2.737E-08
33	6	6	1	6.218E-08
34	1	1	5	1.804E-07
35	3	1	1	6.695E-08
36	6	1	6	2.314E-08
37	6	1	1	3.742E-08
38	1	6	1	8.991E-09
39	3	6	1	7.654E-08
40	5	6	6	1.909E-07
41	1	6	5	1.782E-07
42	7	6	1	4.552E-07

Table 3.7 Continued: DACOS results targeting neutron scalar flux of 1.224x10^{-5} in 3D AGENT UUTR CI by altering B-ring materials

Iteration #	Cell 1 (B2)	Cell 2 (B4)	Cell 3 (B6)	Obj. Fn
43	6	1	3	1.023E-07
44	1	10	6	5.460E-07
45	7	1	1	4.514E-07
46	3	1	10	3.648E-07
47	10	6	6	2.790E-07

Table 3.8: DACOS results targeting k_{eff} of 1.000 in 3D AGENT UUTR by altering shim control rod withdrawn percentage

coliny_ea Results

Iteration #	"shim" rod withdrawn	k_{eff}	Obj. Fn
1	13.3%	0.99482	5.180E-03
2	80.0%	1.00488	4.877E-03
3	40.0%	0.99791	2.086E-03
4	46.7%	0.99913	8.683E-04
5	53.3%	1.00042	4.182E-04
6	86.7%	1.00558	5.579E-03
7	60.0%	1.00170	1.698E-03
8	33.3%	0.99683	3.168E-03
9	26.7%	0.99594	4.059E-03
10	20.0%	0.99527	4.731E-03

SOGA Results

Iteration #	"shim" rod withdrawn	k_{eff}	Obj. Fn
1	6.7%	0.99456	5.439E-03
2	66.7%	1.00290	2.904E-03
3	86.7%	1.00558	5.579E-03
4	93.3%	1.00607	6.075E-03
5	53.3%	1.00042	4.182E-04
6	40.0%	0.99791	2.086E-03
7	20.0%	0.99527	4.731E-03
8	46.7%	0.99913	8.683E-04
9	33.3%	0.99683	3.168E-03
10	60.0%	1.00170	1.698E-03
11	80.0%	1.00488	4.877E-03
12	100.0%	1.00638	6.383E-03
13	26.7%	0.99594	4.059E-03

CHAPTER 4

ENGINEERING SAFETY CULTURE WORKFLOW[1]

4.1 Safety Culture Background

Nuclear research reactors have been used in over 60 countries for approximately 60 years presenting unique and crucial tools in contributing to continuous scientific and engineering advancements. Nuclear research reactors are managed by many different companies, universities, and research centers worldwide. Most nuclear research reactors do not have the large staff and support roles that are commonly found in nuclear power plants. As a result of minimal staffing at most nuclear research reactors, some of the best practices and programs that have been proven at nuclear power plants have not been implemented. An example of this is a lack of a strong nuclear safety culture program toward facility management and operation, and training and education of a new nuclear workforce.

The term "safety culture" has been used in the nuclear industry since the investigation of the Chernobyl Power Plant accident in 1986 by the International Atomic Energy Agency (IAEA) [12]. The U.S. Nuclear Regulatory Commission (NRC) has been monitoring, collecting data, and measuring safety culture indicators at nuclear power plants since the 1980s. In 2011, the NRC released a Safety Culture Policy Statement

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[1] The content for this chapter is based upon research published in conference proceedings, IAEA Technical Meetings, and invited talks [1]-[11].

setting forth the expectation that individuals and organizations establish and maintain a positive safety culture commensurate with their safety and security significance. The NRC defined nuclear safety culture as "*the core values and behaviors resulting from a collective commitment by leaders and individuals to emphasize safety over competing goals to ensure protection of people and the environment*" [13]. The NRC's policy statement is not a regulation or enforceable but guides the activities of the NRC staff and sets forth related expectations. Security at nuclear facilities is an integral part of the safety culture and together they strengthen each other to reduce risk.

There has been no documentation on implementing and studying the impacts of improving the nuclear safety culture at nuclear research reactor facilities in the United States. Recent work has been initiated and numerous studies have been implemented in finding the best practices in safety culture applicable to the nuclear research facility at the Utah Nuclear Engineering Program (UNEP). The newly developed Engineering Safety Culture platform and workflow process is presented with some illustrative examples implemented at UNEP.

4.2 Safety Culture

4.2.1 Engineering Safety Culture (ESC)

Culture is an abstract term used by many different individuals and groups with varied meanings. In order to establish a similar starting point, culture needs to be defined. Schein's [14] formal definition of culture is a broadly accepted model and is used as the starting point in expanding on the Engineering Safety Culture and then further on nuclear safety culture as shown in this paper. "The culture of a group can now be defined as a pattern of shared basic assumptions learned by a group as its problems of external adaptation and internal integration, which has worked well enough to be considered valid and, therefore, to be taught to new members as the correct way to perceive, think, and feel in relation to those problems" [14]. With this definition of a culture in general, the connection between the Engineering Safety Culture and the culture in general is derived and discussed as follows.

As was stated previously, "safety culture" and "nuclear safety culture" are heavily used by the nuclear industry but *Engineering Safety Culture* is a new paradigm and cultural process that is not just limited to the nuclear safety culture at the reactor facilities but to include all aspects of safety culture including the "nuclear safety culture" aspect. *Engineering Safety Culture* is a term that combines both Schein's definition of culture along with the NRC definition of nuclear safety culture and also includes Goble and Bier's [15] ideas on rethinking nuclear emergency planning, preparations and response. Goble and Bier recommend the nuclear industry move from a "culture of safety" to a "culture of protection" and also towards "resilience." The "culture of protection" is inclusive of the entire system with technology, human behavior and the environmental context.

UNEP's definition of *Engineering Safety Culture* is the core values and behaviors resulting from a collective commitment by leaders and individuals to emphasize safety of the entire system over competing goals and in being proactive and adaptive when confronted with disruptions, change, and pressures [4], [8]. The "entire system" in the definition means that it not only includes the components of the reactor and the supporting plant but it also includes the response of those working at the facility but also the response of the public and those that surround the facility. Including the detail of all components surrounding the facility helps ensure a more proactive and adaptive nature of the system to ensure that it can respond to any change and pressure.

4.2.2 The second decade 21st century's issues related to Engineering Safety Culture

In February 2016, the Nuclear Energy Institute (NEI) [16] presented a new initiative titled "Delivering the Nuclear Promise: Advancing Safety, Reliability and Economic Performance." This is a multiyear strategy to help nuclear power plants improve efficiency, to improve operations and reduce electric generating costs. The U.S. Nuclear Power Plant (NPP) industry is facing early closures of NPPs due to many different factors. This NEI initiative has been put in place to help address the current status of NPPs.

To draw parallels to another industry, NASA experienced similar pressures in the late 1990s and early 2000s timeframes. NASA was experiencing pressure to be "faster, better, and cheaper." As a result of these pressures, management was led to decisions that thrust their organization closer to the threshold of the performance envelope without them realizing how risk had increased. This in turn resulted in the 2003 Columbia space shuttle accident [17].

The nuclear industry must be vigilant and cautious while endeavoring in the NEI initiative to "Deliver the Nuclear Promise." The Engineering Safety Culture concept of being proactive and adaptive when confronted with disruptions, change, and pressures is essential. Education and training resulting from this process will aid in ensuring there are individuals that have been indoctrinated in the Engineering Safety Culture concept that are entering the nuclear industry. Engineering Safety Culture plays a vital role in handling and managing the aging research reactor issues.

4.3 Aging research reactors in the world

4.3.1 Worldwide research reactors

The today aging research reactor fleet was predominantly built in the 1960s and 1970s. The 2016 geographic distribution of research reactors is shown in Figure 4.1. These operating research reactors face a variety and complexity of challenges due to the impact of component and system aging.

Under normal operational conditions, research reactor components are exposed to different levels of radiation, temperature or pressure that impact the physical properties of the materials [18]. The IAEA has compiled and analyzed the aging mechanisms that have been sources of research reactor issues. The radiation, corrosion, and cycling are the leading causes of aging research reactor problems from the summaries [19]. Common issues that arise from ageing components can be seen as tracked by the Vienna, Austria TRIGA Mark II reactor [20]. Villa tracked approximately ~4,500 reactor events over a 47-year period and it was determined that 54% of the issues were due to problems with the instrumentation and controls portion of the reactor. The instrumentation and control electronics are sensitive to the aging mechanisms and also become obsolete due to the rapid advancement of technologies and components. The same trends have been seen at the UUTR.

4.3.2 The University of Utah Research Reactor (UUTR)

The UUTR is a Mark I TRIGA open pool type reactor. Construction on the UUTR began in 1972 with the first critical operation in October of 1975. In 1991, a new reactor control console was installed but since then minimal work has been completed on the reactor instrument and control systems. As of July 2017, the UUTR has operated for a total of 3,975 h at a nominal power of 90 kWth. In recent years, numerous operational issues directly related to aging of the reactor components have required emergency repairs under complex conditions (limited space, strict regulations, lack of historical data). These unscheduled repair activities created a significant disruption to facility operations, disrupting both student training and class activities and research schedules. Thus, the UUTR became a driver to develop a synergistic approach to safety culture platform integrating multilevel factors framework in addressing simultaneous issues and operational conditions.

4.4 Paradigm shift in Engineering Safety Culture practices

4.4.1 A research reactor's transformation in education and training leading to a paradigm shift

In the fall of 2009, UNEP began a dramatic transformation of the program in both educational philosophy and training and research curriculum [3], [21]. The curriculum of the program was expanded to include an undergraduate minor in nuclear engineering and was approved by the Utah Board of Regents in May of 2010 [22]. Also, in 2010, a nuclear reactor operator training program was established and prepares student and staff to obtain licenses from the NRC to operate the UUTR. Lastly, in 2010, the graduate program curriculum was advanced to meet the challenges of the 21st century nuclear industry.

With these vast changes in the curriculum and design of the program it also was determined that an Engineering Safety Culture paradigm is missing; the new unique safety culture platform was then established in 2012 that intertwined into and became an integral part of every-day operation, laboratory activities, exercises, research, training, and experiments. A corrective action program (CAP) was developed as an integral part of the established UNEP new Engineering Safety Culture [1]. In that respect, UNEP partnered with DevonWay Company and began using their software called “Track & Trace” to implement a corrective action tracking program [22]. DevonWay software is in use by over 80% of the nuclear power plants and other industries in the United States, to meet their CAP needs. The software is web-based user-centric and is hosted by DevonWay in its certified data center. The UNEP version of this software is used to track purchasing and maintenance processes, education and training of new nuclear force attending classes, and training operational classes at UNEP research reactor facility. Most users are able to quickly and easily grasp navigating and using the DevonWay software. Because DevonWay is cloud-based, accessing the software can be completed from various locations and reports can be retrieved easily [3]. Figure 4.2 demonstrates how integral the CAP program is to the Engineering Safety Culture platform. The UNEP Engineering Safety Culture platform as detailed in Figure 4.2 is patterned after the Nuclear Energy Institute (NEI) task force recommendations given in NEI 09-07, fostering a strong nuclear safety culture [23].

The main purpose of the workflow process shown in Figure 4.2 is to provide a timely indication of possible problems, develop effective corrective actions and monitor effectiveness of the actions taken. The process inputs collect data such as deficiencies, violations, or weaknesses from different mechanisms such as inspections, audits, and assessments and combines them in the CAP:

- **NRC Inspection Results** – UNEP is regulated by the US NRC and as such has NRC inspections of the reactor and processes at a minimum of every two years. These inspections can provide valuable insights with respect to the facility safety culture and its practices.
- **Nuclear Safety Culture Assessment** – UNEP conducts a nuclear safety culture assessment biennially which normally consists of a self-assessment using questionnaires and surveys given to staff and students.
- **RSC Evaluations** – The Reactor Safety Committee (RSC) is required per the regulatory technical specifications and is made up of knowledgeable individuals in the nuclear reactor field both outside of and within the university. The RSC has the primary function to review, audit and approve safety aspects associated with the operation and use of the facility.
- **Operating Experience** – Information from previous problems and issues (such as operations, design, and equipment) are used to improve procedures and processes and avoid future problems.
- **Self-Assessment / Benchmarking** – UNEP staff members audit and review various process and procedures throughout the operations cycle. This information along with information obtained when staff members visit other research reactor facilities is input in to the CAP system for improvements in facility Engineering

Safety Culture.

All of the problems and deficiencies as found in the above process inputs are fed into the DevonWay CAP where they are assessed for significance and prioritized. The improvement items to address or fix the related issues are then tracked to completion in the CAP. The CAP software is available to the RSC which can then monitor the inputs that are indicative of potential problems associated with the Engineering Safety Culture. The RSC reports to the Vice President (VP) for Research at the University of Utah. The VP for Research has the ultimate responsibility for the reactor and has the holistic view of all of the potential indications of Engineering Safety Culture.

The UNEP response to address various Engineering Safety Culture issues could include changes in policies, program modifications, training, additional assessments, etc. The responses also provide feedback into the process inputs and the CAP. It is also important that the actions taken and its conclusions are communicated to the internal and external stakeholders, staff and students as appropriate. This ensures that the individuals providing inputs into the system have positive reinforcement for their efforts and that their voice matters. The external review is conducted by an Industrial Advisory Board (IAB) that is made up of professionals from various companies and government agencies related to the nuclear industry.

4.4.2 INPO and NRC nuclear safety culture traits

The NRC has determined that certain and specific personnel and organizational traits are found in strong nuclear safety cultures. These organizational traits are a pattern of behaviors and ideas that stress safety, particularly in goal conflict situations, over schedule, production and cost [13]. The Institute of Nuclear Power Operations (INPO) took the policy statement from the NRC, guiding documents from the International Atomic Energy Agency [24], and input from the nuclear industry to generate a list of traits of the well-specified healthy nuclear safety culture [25]. UNEP has implemented these traits into all training, research, classroom, and laboratories. Table 4.1 lists these traits following the INPO 12-012 categories:

- **Individual Commitment to Safety** – This category defines and guides how every individual that interfaces with the facility is dedicated to the framework of safety that has been provided by the leadership team. Even with the best safety programs, if the individuals do not internalize the concepts, a safer environment will not be achieved. The specific components defining and building individual commitment to safety are:
    - ***Personal Accountability (PA)*** – All individuals recognize and take personal responsibility for safety and understand the significance of adherence to facility standards and procedures. Each person takes ownership for his/her actions and how he/she impacts the overall safety.
    - ***Questioning Attitude (QA)*** – A questioning attitude fosters awareness of uncertainty, hazards, and the significance of an action or series of actions before proceeding. Individuals avoid complacency and continuously challenge existing conditions and activities in order to identify discrepancies.
    - ***Effective Safety Communication (CO)*** – Communications maintain a focus on safety. Individuals frequently converse with each other in an open, courteous manner, they are also more prepared to give and receive feedback.
- **Management Commitment to Safety** – In order for individuals to carry out the

individual traits, the leadership or management of the facility must emulate the characters for individuals but also create environments that foster attitudes conducive to safety:

- ***Leadership Safety Values and Actions (LA)*** – Leaders display and express a commitment to safety in their decisions and behaviors. The leaders have a significant impact on the organizations Engineering Safety Culture through the priorities that the leaders establish, values and behaviors they model, and the reward system they administer.
- ***Decision-Making (DM)*** – Decisions that encourage or affect Engineering Safety Culture are methodical, rigorous, and detailed. Leaders also use conservative concepts of decision-making and emphasize prudent choices.
- ***Respectful Work Environment (WE)*** – Trust and respect permeate the facility and program. Trust and respect instill confidence that the facility and program is just and fair, promoting open communications and accurate reporting.

- **Management Systems** – The policies, procedures and programs that cultivate and enhance the overall emphasis on safety.
  - ***Continuous Learning (CL)*** – Opportunities to learn about ways to ensure safety are pursued and applied. This trait features learning from mistakes and those of others and then implementing the lessons learned to prevent further errors.
  - ***Problem Identification and Resolution (PI)*** – Problems possibly impacting safety are quickly identified, completely assessed, and promptly addressed and corrected commensurate with their importance.
  - ***Environment for Raising Concerns (RC)*** – A safety-conscious work

environment (SCWE) is supported where individuals feel free to raise safety concerns without apprehension of retaliation, intimidation, harassment, or discrimination.

- ***Work Processes (WP)*** – The process of scheduling and monitoring work activities is executed so that safety is upheld.

4.4.3 Examples of applying the Engineering Safety Culture traits

The safety traits as listed in Table 4.1 and described in Section 4.3.2, were implemented into the everyday fabric of the UNEP Program education and training curriculum; details and examples of its implementation are described as follows:

- **Individual Commitment to Safety at UNEP**
  - ***Personal Accountability (PA)*** – All individuals conducting research or completing work in the UNEP facilities must complete the dynamic learning activity (DLA) that is implemented at the beginning of each semester [5]. The DLA contains training on the Engineering Safety Culture concept, human performance error reduction techniques, coaching and correcting others, and an interactive activity in identification of hazards. The DLA training introduces individuals to the concept of personal/individual responsibility to individual and group safety, as well as facility safety.
    - *UNEP Implementation* – UNEP staff members have rewritten operating procedures that for the first time included initialing and signing for procedural and process steps instead of just check marks. Specifically, the UUTR startup and monthly surveillance procedures were updated from simple one-page check

sheets to formal procedures requiring steps to be initialed by the performer and signatures by licensed operators. This gave individuals personal accountability for completing procedures.

- ***Questioning Attitude (QA)*** – Research review meetings, self-assessment, classes and laboratories conducted at UNEP always include encouragement of students to question **why** and challenge the unknown and assumptions given.
  - *UNEP Implementation* – During a self-assessment of the UNEP Radiation Protection Program, an individual questioned the calculation being conducted in the monthly surveillance procedure to determine the radioisotope levels in the reactor tank water. The procedure gave directions to sample the water but was not clear on sample amount and acceptance criteria. The technical basis for the procedural step could not be identified. The questioning attitude of the individual resulted in acceptance criteria being developed for the radioisotope water level and clear directions on sample size and calculations.
- ***Effective Safety Communication (CO)*** – As part of the introductory DLA for all individuals, a roleplaying interactive example of correcting and coaching is conducted at the beginning of each University semester. This introduces and allows individuals to practice and become comfortable with safety communications.
  - *UNEP Implementation* – UNEP is utilizing social media to enhance and build on the various traits of a healthy Engineering Safety Culture [5]. This allows safety related communication to be sent to all those involved in a timely, frequent, and accurate manner.

- **Management Commitment to Safety at UNEP**
  - ***Leadership Safety Values and Actions (LA)*** – The leadership of UNEP is responsible for the implementation and changes that have occurred since 2009 and have implemented the procedures and programs presented in this paper.
    - *UNEP Implementation* – The leadership at UNEP, comprising the University of Utah Vice President for Research, UNEP Director, and UNEP Reactor Supervisor, has worked tirelessly with the RSC to make the changes discussed from 2009 to the present. A specific example of this is the UNEP leadership devoting the resources and time for the first lab and class of each semester to performing the safety DLA. This sets the tone for all students and staff that safety is of the upmost importance.
  - ***Decision-Making (DM)*** – UNEP staff and leaders take a conservative approach to decision-making, specifically when information is incomplete, or conditions are abnormal.
    - *UNEP Implementation* – Leadership at UNEP made the decision to cancel scheduled laboratories that involved reactor operation when an unusual condition was found during the prestartup checks reflecting a conservative decision-making mindset. In February 2016, while conducting a reactor power operation run, the log power indications for the UUTR did not respond as expected. The log power is not required per the regulatory technical specifications of the U.S. NRC but is a useful indication of reactor power for operators and also gives the indication for reactor period. UNEP leadership cancelled the previously planned classes and laboratories that included reactor

operations while log power was investigated.

- ***Respectful Work Environment (WE)*** – UNEP works to instill the highest levels of trust amongst researchers, staff and students. All individuals are encouraged to voice concerns or differences of opinions in all training and teaching environments.
  - *UNEP Implementation* – UNEP has established a reward system that recognizes individuals for identifying deficiencies and inputting the deficiency into the CAP. The reward system is named "Utahnium" and was initially implemented in January 2016. When students identify a safety hazard and input it into the CAP they are then recognized in front of their peers and are awarded "Utahnium" points. When three points are reached by a student they receive additional prizes and are recognized as a "Utahnium Ambassador." Student have responded well to the positive reinforcement and are making a positive impact on improving the safety of the facility.

- **Management System at UNEP**
  - ***Continuous Learning (CL)*** – UNEP evaluates its programs and policies for opportunities for improvement, benchmark other organizations, and understand the importance of training. UNEP ensures that opportunities to improve safety are identified and shared, and by doing so, builds a strong Engineering Safety Culture.
    - *UNEP Implementation* – UNEP has begun extensive internal self-assessments by staff on their emergency response procedures resulting in multiple improvements in both procedures and training. In May 2014, the Reactor

Supervisor conducted as self-assessment of the Emergency Plan and identified that the memorandum of agreements for ambulance coverage had not been updated for over 20 years. The ambulance provider was contacted and new updated memorandum of agreements were established for UNEP and the ambulance provider.

- ***Problem Identification and Resolution (PI)*** – With the recent implementation of the DevonWay CAP UNEP now has the ability and willingness of staff and students to identify and address problems. The problems are also tracked and monitored for resolution.
  - *UNEP Implementation* – For example, UNEP staff have identified issues related to security systems that were clearly identified and presented to NRC inspectors and in turn tracked to resolution in repairing and addressing the cause of the failures.
- ***Environment for Raising Concerns (RC)*** – UNEP has implemented a policy that supports individuals' rights and responsibilities to raise safety concerns and does not tolerate harassment, intimidation, retaliation, or discrimination for doing so. Senior leaders have an open-door policy for raising concerns as well.
  - *UNEP Implementation* – The VP for Research at the University of Utah has established clear communications that any individual can raise concerns to their office if any individuals feel the need to raise the concern confidentially.
- ***Work Processes (WP)*** – UNEP has modified and updated work procedures to make them complete, accurate, and up-to-date. Historically, it was difficult to track and obtain accurate and thorough documentation of maintenance and

repairs.

- *UNEP Implementation* – The RSC has commented in official meeting minutes how easily it has been to track and follow maintenance and repairs that have been conducted due to the high-quality work documentation and process.

4.5 Engineering Safety Culture ideology and process

4.5.1 The Engineering Safety Culture workflow process explanation

A new process of how to efficiently address and work through anything from incidents and accidents to implementing new ideas from staff members or students using the new Engineering Safety Culture (ESC) process has been developed and given in Figure 4.3. This is the ideology that should be ingrained and followed for an effective ESC to be in place at any facility. It begins with the importance that was emphasized in the healthy nuclear safety culture traits of everyone is responsible and identifies issues or improvements. This process depends upon the *identification* stage. If the individuals working in the facility are not encouraged and feel value is given for their efforts of identifying deficiencies, problems or new improvement ideas, this process will not function correctly.

After individuals come forward with the problem or idea the importance of *taking immediate action* is vital. All individuals should be trained to ensure immediate action is taken to place equipment, processes, or people in a safe condition and remove all hazards. It is also important that personnel that have been trained and/or licensed are *notified* of the hazards or conditions that could have an impact on licenses or operations.

Once the proper operational supervisor has been *notified*, the problem must be *documented* in the corrective action program (CAP). This is where the process is intertwined with Figure 4.2. An idea or improvement action is now tracked and followed in the CAP. This allows for the likelihood that an action will be taken due to it being recorded and reviewed by supervisors. At research reactor facilities, it is common for good ideas to come forward but not be documented and in turn not be completed. *Documentation* is an important part of the ESC process.

Certain issues, problems, or changes require that the oversight or regulator be *contacted* within specific time frames. Changes with regard to license structures, systems, components, or processes also must be tracked following the regulators guidelines such as the 10 CFR 50.59 process with the United States Nuclear Regulatory Commission (U.S. NRC). This *determination* of change management ensures the proper resources are devoted.

The operational staff must *evaluate*, using the healthy nuclear safety culture traits, and prioritize the actions taken and resources allocated to fix, develop processes, or address the issue or new idea. Figure 4.3 shows the three different levels of prioritization. High priority items, Level 1 ESC, are those that can impact immediate operations or safety. These must be given immediate resources to take care of the issue or event identified. Level 2 ESC should be given adequate resources and effort due to the potential for safety or operational impact. Level 3 ESC are most likely ideas or processes that can improve the overall operations and safety but do not impact current operations and safety.

After the appropriate ESC level has been determined, *assignment, actions, and deadlines* are given to ensure completion. Once the actions have been take and completed, an *assessment* is conducted to see if the actions have adequately addressed the identified issue or idea. If they have not been addressed appropriately, the issue is fed back to the *evaluatio*n part of the process. *Communicating* the actions taken both before actions are taken and after is important so that individual contributors can see their efforts are bringing about change. If the communications don't occur, individuals could lose interest in the process of improvement which could result in less inputs to the identification stage.

The final *documentation* in the CAP ensures that future actions taken or issues that happen related to the actions can be researched and found. This also ensures that as individuals leave or turn over, a continuity of improvement is retained.

4.5.2 Case studies examples of the Engineering Safety Culture process implementation at UNEP

4.5.2.1 Reduction in unplanned reactor shutdowns (SCRAMs)

This case study demonstrates the personal accountability (PA), questioning attitude (QA), effective safety communication (CO), decision-making (DM), and problem identification and resolution (PI) among the traits listed in Table 4.1. The Figure 4.3 ESC workflow process is also demonstrated.

In July of 2013, during a reactor operation, an automatic shutdown (SCRAM) occurred due to the control system indicating a lowering tank water level. The issue was *identified* of an unplanned shutdown occurring. The water level SCRAM is required to ensure enough radiological shielding, the reactor tank water, is in place to protect people and the environment. If water level drops below the given set-point, proper shielding cannot be ensured. The operators immediately reviewed redundant indication and noted that actual tank water level was not changing.

Immediate action was taken to ensure no hazards or safety problems existed. The operators stopped the operational activities when confronted with an unexpected condition, *notified* the operational supervisors, and worked to resolve the condition prior to continuing operational activities (QA). The low-water-level SCRAM had occurred due to an erroneous water level signal. It was determined that *contacting* the regulator was not required and the oversight committee would be informed at the next quarterly meeting. After *evaluating* and reviewing, previous nuclear reactor operating records it was found that there was a rising trend in the history of erroneous low-water-level SCRAMs at the UUTR. Figure 4.4 shows that in 2010 the UUTR had two erroneous low-water-level SCRAMs followed by two consecutive years of five.

The operational staff assigned Level 1 ESC high priority resources for the water level issue. Midway through the year in 2013 *assignments* were made and repairs were conducted on the electronics. Four erroneous low-water-level SCRAMs had already happened in the first half of 2013 with a projected four more expected had no repairs occurred. The actions taken to repair the low-water-level circuitry were *assessed* and no erroneous low-water-level SCRAMs have occurred in the following three years (2014-2016). All actions and repairs were meticulously *documented* in the CAP including pictures and schematics. Finally, the actions taken and the positive results were *communicated* out to facility staff and students via the facility website and social media. This case study demonstrates that the ESC workflow process has had a positive impact on improving reliable operations of the UUTR at UNEP.

4.5.2.2 Fuel inspection device development

The need for a designed fuel inspection device example displays the Table 4.1 traits of a respectful work environment (WE) and continuous learning (CL) and also demonstrates the Figure 4.3 ESC process being implemented on a new idea and process improvement instead of a failure or incident.

For the life of the UUTR, a technical specification requirement has been in place to inspect each fuel element every two years. Part of the inspection is to ensure that each fuel rod has not developed too large of a specified bend or elongated past the original length a certain amount. This requirement ensures that the fuel is not damaged and operational. The original thought process of UNEP staff was that if the fuel rod fit back into the upper and lower grid plates in the core, the fuel rod did not exceed the transverse bend or elongation license requirements.

Demonstrating a strong respectful work environment (WE) where individuals are encouraged to offer ideas, concerns and suggestions; staff members raised the concern about fuel measurement and *identified* a better and more precise method to measure the fuel rods to ensure safe reactor operation.

No *immediate action* was necessary and the operational supervisor was *notified* of the process improvement for a fuel inspection device. The oversight and regulators did not need to be *contacted* and it was *determined* that the change process would be considered. The operational staff *evaluated* the new idea and assigned to it a Level 3 ESC priority. Students and staff were *assigned* with designing a better fuel rod measurement technique. The continuous learning (CL) attribute of benchmarking was used in gathering information from other research reactors on what methods they were using to measure the fuel rods. It was decided upon that a go-no-go type device be designed and built that each fuel element would be placed in during fuel inspections. The inside diameter is such that if the fuel element fits inside freely it has not exceeded the transverse bend requirement. The top funnel was designed with a viewing window with graduated marks to measure the length of the fuel rod.

A more robust fuel inspection is now being conducted on the UUTR with the new fuel inspection device. The fuel inspection device was utilized in the most recent biennial fuel inspection conducted in May 2016 at the UUTR. The new fuel inspection device was *assessed* after conducting the fuel inspection and no additional actions were warranted. For the first time since construction of the reactor, each fuel rod has been measured and documented, improving the safety and thus demonstrating the benefits of implementing the ESC workflow process.

4.6 References

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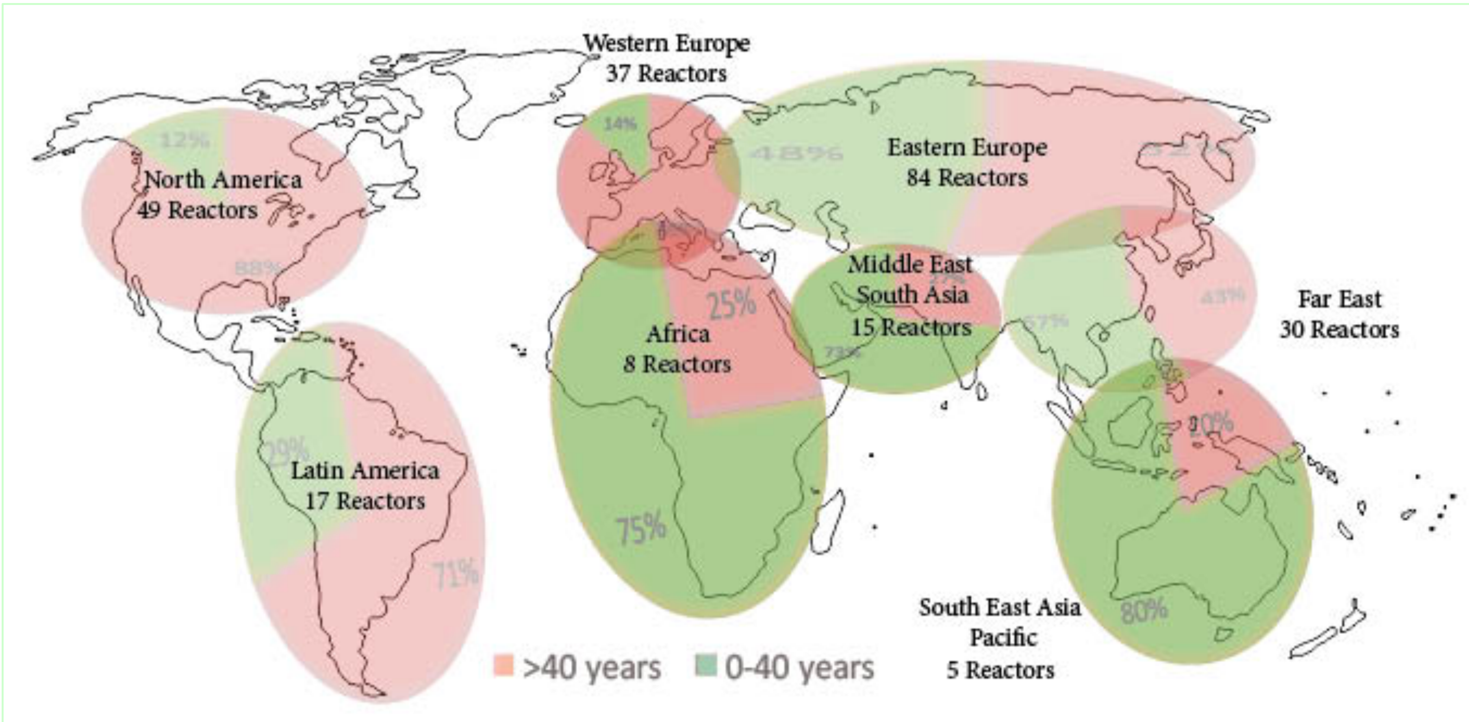

Figure 4.1: 2016 world research reactor geographic distribution with reactor age [out of the 243 operational research reactors in the world 124 operate at a lower power level than 100 kWth with the largest research reactors operating at a maximum power of 20 to 250 MWth]

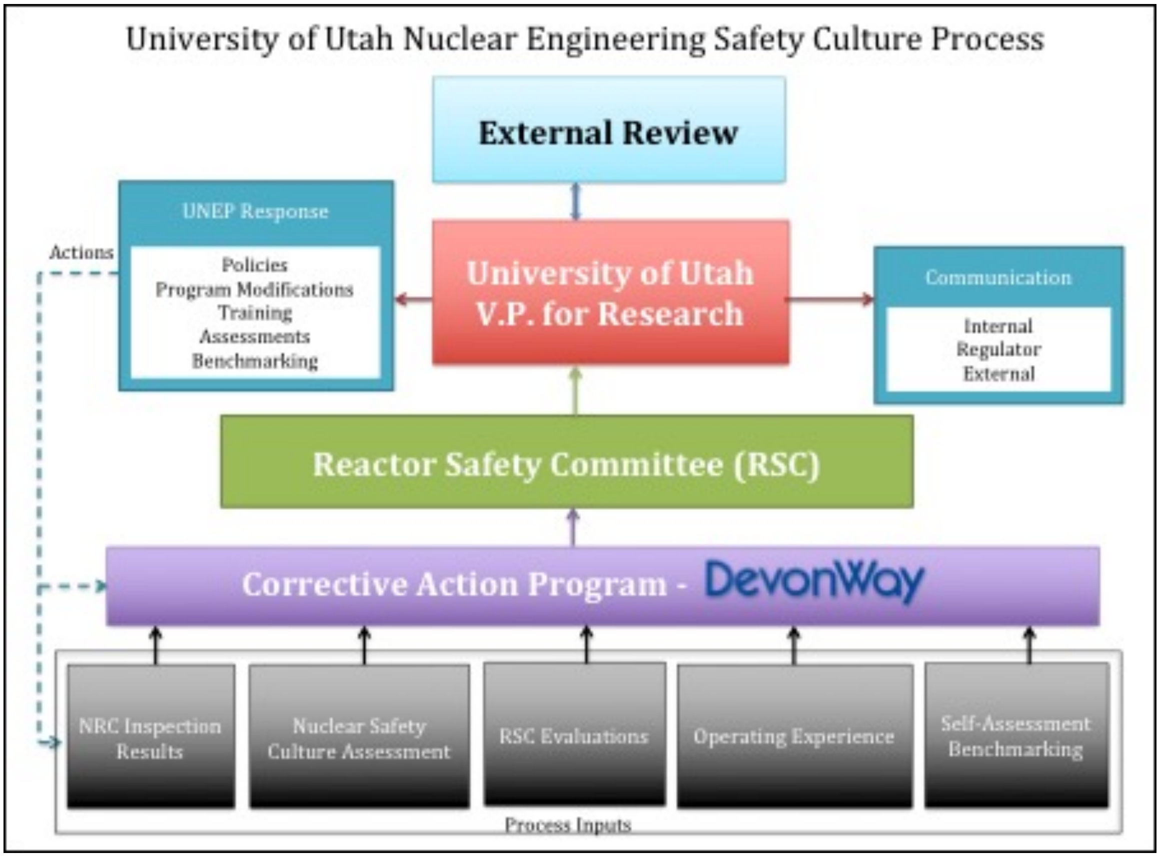

Figure 4.2: UNEP Engineering Safety Culture flowchart of responsibilities and workflow

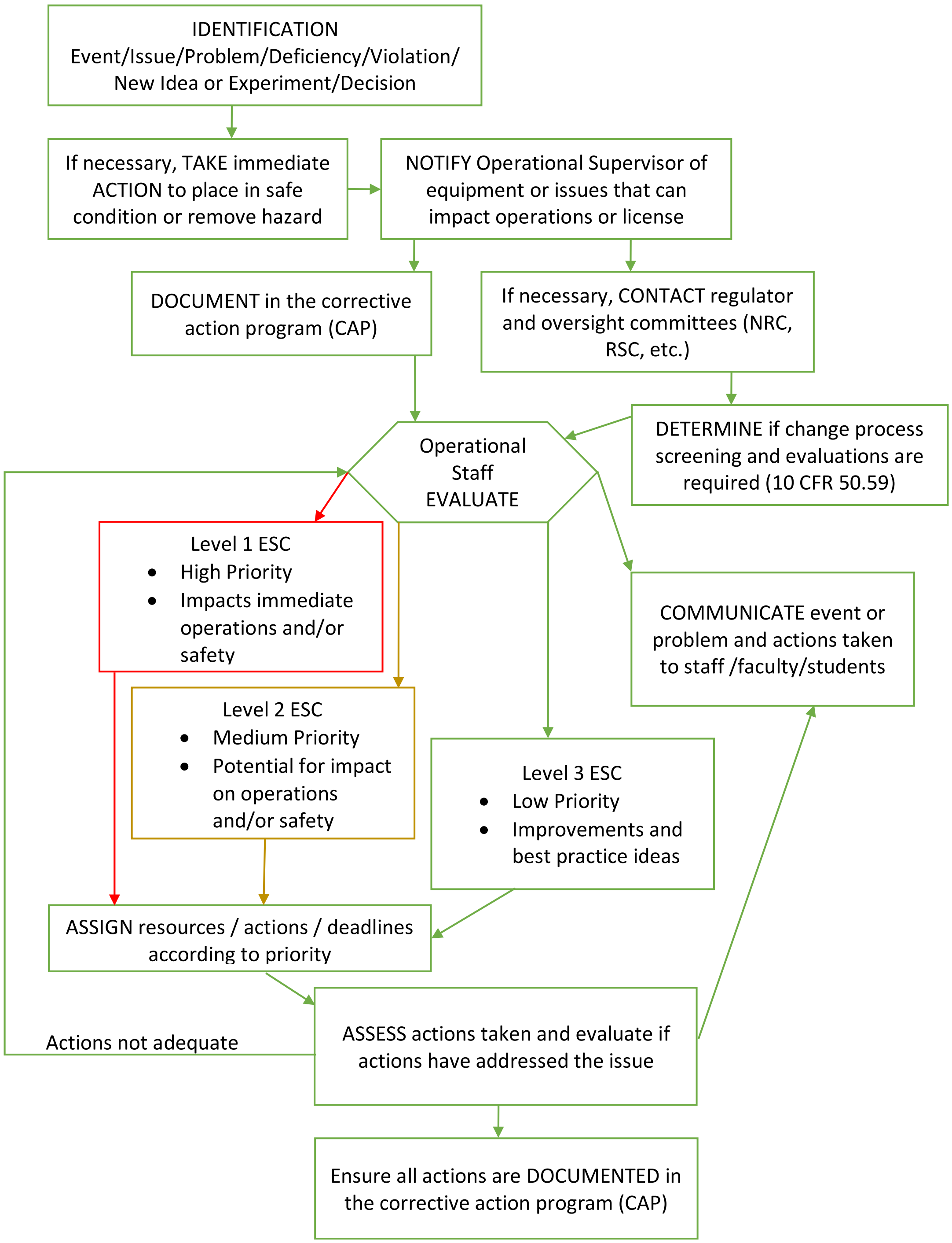

Figure 4.3: Engineering Safety Culture workflow process for all facility issues and ideas

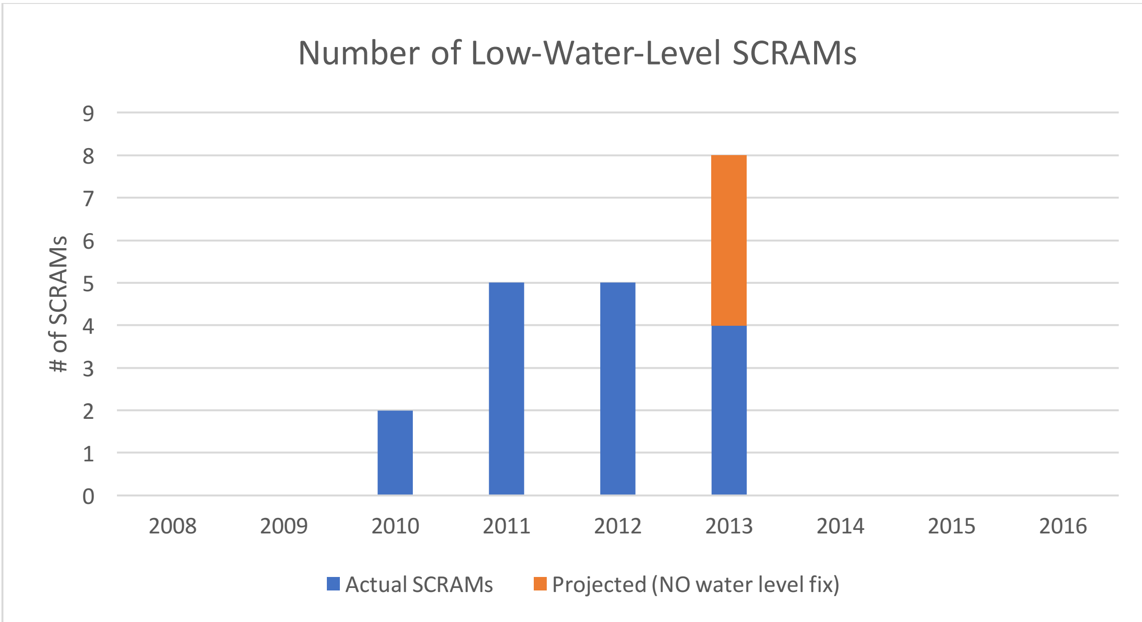

Figure 4.4: Low-water-level SCRAMs at the UUTR from 2008-2016

Table 4.1: INPO traits of a healthy Nuclear Safety Culture

Individual Commitment to Safety	**Management Commitment to Safety**	**Management Systems**
Personal Accountability (PA)	Leadership Safety Values and Actions (LA)	Continuous Learning (CL)
Questioning Attitude (QA)	Decision-Making (DM)	Problem Identification and Resolution (PI)
Effective Safety Communication (CO)	Respectful Work Environment (WE)	Environment for Raising Concerns (RC)
		Work Processes (WP)

CHAPTER 5

CONCLUSIONS AND FUTURE WORK

5.1 Conclusion

The aging research reactors throughout the world are in need of new innovative methodologies to keep them running safety and efficiently. A novel multilevel safety factors-centered framework that can address and fix the aging and inefficient mechanisms of research reactor operations has been given in this dissertation. The framework is housed within an overarching strong Engineering Safety Culture program that encompasses the optimization of experiments such as neutron activation analysis (NAA) and the reactor operational parameters.

NAA is used by many researchers and scientists to determine the elemental properties of various samples. Engineering Safety Culture, regulations, and good practices, necessitate that facilities try to activate as little materials as possible and maintain ALARA. This is in competition with activating target nuclides to high enough activities to also measure the activity with given laboratory equipment and procedures (≥MDL). It is recommended that the optimal NAA parameters such as irradiation time, sample size, neutron flux (reactor port and power level), and counting delay time can be determined prior to the actual conduct of the NAA using the coupling of an optimization code, DAKOTA, with a neutron interaction calculator, PyNIC. The PyNIC-DAKOTA tool system was successful in obtaining the optimal experimental parameters for conducting NAA at research reactors [1]. The PyNIC-DAKOTA tool system was demonstrated with both cobalt and coal fly ash irradiation examples conducted at the UUTR. The results indicated that the PyNIC-DAKOTA system was capable of finding the optimal experimental parameters for NAA with slight variations from the experiments. The PyNIC-DAKOTA tool has been shown to enhance the nuclear safety at the facility by minimizing dose and radiation waste products. This method could be applied at any research reactor facility to optimally determine the parameters for running NAA and improve the nuclear safety.

A novel neutronic optimization system was developed by coupling the neutronics code system, AGENT, with the adaptable optimization software, DAKOTA, to form the DAKOTA-AGENT Computational Optimization System (DACOS) [2]. The DACOS can be related to any nuclear reactor design for optimizing the required parameters such as but not limited to power level, reactor fuel distribution and enrichment, and control rod positions. DAKOTA's optimization algorithms are robust and incorporate well with AGENT. Two genetic algorithms from DAKOTA's library, SOGA and coliny_ea, were applied and compared within the DACOS for some representative benchmark examples. The benchmark examples were developed for the UUTR. The DACOS was tested for the arrangement of core materials in order to obtain k_{eff}, specific neutron flux and/or reactor power values. The DACOS was also used to alter the amount of rod withdrawal in the UUTR to obtain a given k_{eff}. Results from the DACOS benchmarks were compared to MCNP calculations of the UUTR in showing expected agreement. The DACOS is flexible in that it can be used for any type of a reactor of any level of complexity including also the large power reactors. The DACOS enhances the Engineering Safety Culture at nuclear reactor facilities by ensuring accurate and efficient information for rearrangement and design of new fuel systems.

The implementation and ideology of a strong Engineering Safety Culture program results in many benefits and enhancements at a university research reactor. Many long standing and acceptable mediocre equipment and methods of operation can be fixed or addressed due to the traits of a healthy Engineering Safety Culture. An overall Engineering Safety Culture factor centered framework is presented and the working details of how that improves both operational reliability, safety and efficiency. Currently the nuclear industry is feeling the pressure to become “faster, better, and cheaper” with initiatives like NEI’s “Delivering the Nuclear Promise” [3]. The given Engineering Safety Culture factor centered framework implementation at university reactors can provide nuclear professionals to the industry that have been indoctrinated in Engineering Safety Culture to impact the culture of their companies in a positive way and possibly prevent the next nuclear accident.

The Engineering Safety Culture workflow process was developed to work along with the healthy nuclear safety culture traits to improve and enhance operational and safety conditions at any research reactor facility [4]. The Engineering Safety Culture workflow process must be understood by all participants in the facility and integrated into their daily work and thought process. The Engineering Safety Culture workflow process can be used for both addressing incidents and deficiencies as well as introducing new ideas and improvements. Case study examples were given from the UNEP in implementation of the engineering workflow process. Both addressing inadvertent reactor shutdowns and improving reactor fuel inspection examples of the Engineering Safety Culture workflow process were given.

It is also important to point out that the key link of the healthy Engineering Safety Culture, even though it is everyone's responsibility, is based on leadership support and backing. Without the sponsorship and dedication of the leaders and managers, the Engineering Safety Culture would be weak. UNEP has demonstrated the example of improving Engineering Safety Culture due to the leaders reinforcing Engineering Safety Culture at every opportunity and in every environment. Whether it be in the classroom or laboratory, Engineering Safety Culture is intertwined in everything that is done and discussed in the nuclear engineering program. The leadership support is vital for effective and useful implementation of Engineering Safety Culture.

5.2 Future Work

Future work includes continued benchmarking of the PyNIC-DAKOTA tool system to additional NAA experiments including a variety of materials and activities. Benchmark test of the PyNIC-DAKOTA tool system on other research reactors conducting NAA would also demonstrate the capability for the tool to be implemented at any facility. Other potential improvements for the PyNIC-DAKOTA tool would be in making a more user-friendly interface for the PyNIC-DAKOTA tools system, possibly a graphical user interface (GUI), so that end users will not need to have an understanding and knowledge of the python coding and DAKOTA input files. This would allow outside experimenters or students the capability to access the GUI remotely, such as on-line, and determine the experimental NAA parameters. DAKOTA has various genetic algorithms and within each algorithm there are many options such as population size, mutation rate, and cross-over rate. Testing and performance improvement could be conducted on implementing the different genetic algorithms and their associated options on the PyNIC-DAKOTA tool system. Studies on the sensitivity of the various parameter inputs in the PyNIC-DAKOTA tool system and their impact on the objective function could be conducted to further understand the effectiveness and possible utilization of the tool. Implementation of the PyNIC-DAKOTA system for other experimental applications besides NAA could also be investigated such as nuclear fuel interrogation and neutron therapy.

The future use of DACOS is targeted toward optimizing a neutron activation or material irradiation experiments given the UUTR has four different ports available for sample irradiations; equally DACOS can be applied to redesigning the UUTR core in raising its licensed power should that be desired. The DACOS usefulness can be improved immensely by reducing the run time of AGENT. For future DACOS testing of altering the majority of a reactor's materials, AGENT calculation time reductions would make the DACOS tool much more beneficial. Benchmarking the DACOS on other research reactors and nuclear power plants will also be beneficial in improving the operation and accuracy of the DACOS. The different DAKOTA genetic algorithms and their options such as population size and mutation rate also could be tested and optimized for the best implementation in the DACOS. The design of a graphical user interface for users to easily input and obtain results from the DACOS also needs to be developed, tested, and implemented.

Enhancing Engineering Safety Culture is a continuous improvement process wherever it is implemented. Facilities that have begun implementing ideas and processes to improve Engineering Safety Culture must be diligent and vigilant in always evaluating, acting and changing things to improve the process. The ESC must be heavily used and examined when personnel at the facility turnover to ensure that the attitudes and expectations are not lost when individuals change. One aspect of culture and Engineering Safety Culture that has not been achieved is an effective way to measure or evaluate the Engineering Safety Culture. Future work in helping different programs, companies, and universities in improving Engineering Safety Culture begins with how it is measured or evaluated. Participant surveys and anecdotal evidence are the only mechanisms that appear to be used in attempting to evaluate cultures and different facilities. The development of new thought processes and ways to effectively measure and, in turn, give recommendations for improvement on facility and company culture is needed. New and effective mechanisms or programs on changing and improving Engineering Safety Culture are also in demand. A study of how to effectively measure, recommend, and change Engineering Safety Culture would greatly enhance the ability for high risk industries like nuclear power to continue to move forward and have public support and trust.

5.3 References

[1] R. C. Schow and T. Jevremovic, "Optimized neutron activation analysis laboratory-based tool system: PyNIC–DAKOTA," submitted for publication in *Eur. Physical J. - Nucl. Sci. Technol.,* Jun. 2017.

[2] R. C. Schow, D. Kim and T. Jevremovic, "DACOS: DAKOTA-AGENT neutronics computational optimization system," *Ann. Nucl. Energy,* vol. 112, pp. 245-256, Feb. 2018.

[3] Nuclear Energy Institute (NEI), "Delivering the nuclear promise: advancing safety, reliability and economic performance," Washington D.C., USA, 2016.

[4] R. C. Schow and T. Jevremovic, "Enhancing nuclear safety culture training through knowledge management and emergency response exercises," in *NESTet Nucl. Eng. Sci. Technol.*, Berlin, Germany, May 2016.

APPENDIX A

EXAMPLE PyNIC-DAKOTA TOOL SYSTEM INPUT FILE

```
# Demonstrate DAKOTA interface to PyNIC

environment
        tabular_data

method,
          soga
          initialization_type unique_random
          crossover_type shuffle_random
          convergence_tolerance = 1e-4
          print_each_pop

model
        single

variables,
        continuous_design = 3
          initial_point       0.1                2.0                10.0

          upper_bounds        0.3                5                  60

          lower_bounds        0.05               1.0                5
          descriptors        'mass' 'IrrTime' 'DecayTime'
        discrete_design_set
          string = 1
            num_set_values = 14
            set_values = 'CI_90' 'FNIF_90' 'PI_1' 'PI_10' 'PI_30' 'PI_50'
'PI_70' 'PI_90' 'TI_1' 'TI_10' 'TI_30' 'TI_50' 'TI_70' 'TI_90'
            descriptors     'irradPort'

interface,
        fork
          analysis_drivers = 'pynic_bb.py'
          file_tag
          file_save

responses,
        num_objective_functions = 1
        no_hessians
        no_gradients
```

APPENDIX B

EXAMPLE PyNIC-DAKOTA TOOL SYSTEM DATA PRE AND POST PROCESSING FILE – 'pynic_bb.py'

```
#!/usr/bin/env python

# Read DAKOTA parameters file (aprepro or standard format) and call
# PyNIC for analysis.


# DAKOTA will execute this script as
#   pynic_bb.py params.in results.out
# so sys.argv[1] will be the parameters file and
#    sys.argv[2] will be the results file to return to DAKOTA

# necessary python modules
import sys
import re
import os

# ----------------------------
# Parse DAKOTA parameters file
# ----------------------------

# setup regular expressions for parameter/label matching
e = '-?(?:\\d+\\.?\\d*|\\.\\d+)[eEdD](?:\\+|-)?\\d+' # exponential
notation
f = '-?\\d+\\.\\d*|-?\\.\\d+'                          # floating point
i = '-?\\d+'                                            # integer
value = e+'|'+f+'|'+i                                   # numeric field
tag = '\\w+(?::\\w+)*'                                  # text tag field


# regular expression for standard parameters format

standard_regex = re.compile('^\s*(' + value +')\s+(' + tag + ')$')
nonstandard_regex = re.compile('^\s*(' + tag +')\s+(' + tag + ')$')

# open DAKOTA parameters file for reading in CV
paramsfile = open(sys.argv[1], 'r')

# extract the CV parameters from the file and store in a dictionary
paramsdict = {}
for line in paramsfile:
        m = standard_regex.match(line)
        if m:
            paramsdict[m.group(2)] = m.group(1)

paramsfile.close()

# open DAKOTA parameters file for reading in DV
paramsfile = open(sys.argv[1], 'r')

# extract the DV parameters from the file and store in a dictionary
```

```
paramsdictdv = {}
for line in paramsfile:
        m = nonstandard_regex.match(line)
        if m:
            paramsdictdv[m.group(2)] = m.group(1)

paramsfile.close()

# crude error checking; handle both standard and aprepro cases
num_vars = 0
if ('variables' in paramsdict):
    num_vars = int(paramsdict['variables'])
elif ('DAKOTA_VARS' in paramsdict):
    num_vars = int(paramsdict['DAKOTA_VARS'])

num_fns = 0
if ('functions' in paramsdict):
    num_fns = int(paramsdict['functions'])
elif ('DAKOTA_FNS' in paramsdict):
    num_fns = int(paramsdict['DAKOTA_FNS'])

if (num_vars != 4 or num_fns != 1):
    print "PyNIC requires 4 variables and 1 function;\nfound " + \
   str( num_vars) + " variables and " + str(num_fns) + " functions."
    sys.exit(1)

# -------------------------------
# Convert and send to application
# -------------------------------

# set up the data structures the PyNIC analysis code expects
# for this simple example, put all the variables into a single
hardwired array
continuous_vars = [ float(paramsdict['mass']),
float(paramsdict['IrrTime']), float(paramsdict['DecayTime']) ]
discrete_vars = [ str(paramsdictdv['irradPort']) ]
active_set_vector = [ int(paramsdict['ASV_1:obj_fn']) ]

# set a dictionary for passing to PyNIC via Python kwargs
pynic_params = {}
pynic_params['cv'] = continuous_vars
pynic_params['dv'] = discrete_vars
pynic_params['asv'] = active_set_vector
pynic_params['functions'] = 1

# execute the PyNIC analysis as a separate Python module
#print "Running PyNIC..."
from NAA_Report_generator import pynic_list
pynic_results = pynic_list(**pynic_params)
#print "PyNIC complete."
```

```
# ----------------------------
# Return the results to DAKOTA
# ----------------------------

# write the results.out file for return to DAKOTA
# this example only has a single function, so make some assumptions;
# not processing DVV
outfile = open('results.out.tmp', 'w')

# write functions
for func_ind in range(0, num_fns):
    if (active_set_vector[func_ind] & 1):
        functions = pynic_results['fns']
        outfile.write(str(functions) + ' f' + str(func_ind) + '\n')

# write gradients
#for func_ind in range(0, num_fns):
#    if (active_set_vector[func_ind] & 2):
#        grad = pynic_results['fnGrads'][func_ind]
#        outfile.write('[ ')
#        for deriv in grad:
#            outfile.write(str(deriv) + ' ')
#        outfile.write(']\n')

# write Hessians
#for func_ind in range(0, num_fns):
#    if (active_set_vector[func_ind] & 4):
#        hessian = pynic_results['fnHessians'][func_ind]
#        outfile.write('[[ ')
#        for hessrow in hessian:
#            for hesscol in hessrow:
#                outfile.write(str(hesscol) + ' ')
#            outfile.write('\n')
#        outfile.write(']]')

outfile.close()

# move the temporary results file to the one DAKOTA expects
import shutil
shutil.move('results.out.tmp', sys.argv[2])
#os.system('mv results.out.tmp ' + sys.argv[2])
```

APPENDIX C

EXAMPLE DACOS INPUT FILE

```
#  DAKOTA INPUT FILE - dakota_agent.in
#  This sample Dakota input file varies core materials in the UUTR for
multi AGENT.

environment,
    graphics
    tabular_data
    tabular_graphics_file= 'agent_multidim.dat'

method,
    soga
    population_size = 10
    print_each_pop

model,
    single

variables,
    discrete_design_set
    integer = 3
    elements_per_variable = 6 6 6
    elements = 1 3 5 6 7 10 1 3 5 6 7 10 1 3 5 6 7 10
    descriptor = 'cell1' 'cell2' 'cell3'

interface,
        fork
          analysis_driver = 'agent_script'
          parameters_file = 'params.in'
          results_file    = 'dakota_agent.out'
          aprepro
          deactivate active_set_vector
          file_save

responses,
        response_descriptors = 'CI_flux'
        num_objective_functions = 1
        no_gradients
        no_hessians
```

APPENDIX D

EXAMPLE DACOS DATA PRE AND POST PROCESSING

FILE – ‘agent_script’

```
#!/bin/sh
# Sample simulator to Dakota system call script
# See Advanced Simulation Code Interfaces chapter in Users Manual

# $1 is params.in FROM Dakota
# $2 is results.out returned to Dakota

# --------------
# PRE-PROCESSING
# --------------
# Incorporate the parameters from DAKOTA into the template, writing
ros.in
# Use the following line if SNL's APREPRO utility is used instead of
DPrePro.
# ../aprepro -c '*' -q --nowarning ros.template ros.in

dprepro $1 agent.template agent.inp

# --------
# ANALYSIS
#---------

#multi_agent | grep -P 'K-INF = ' | cut -d \= -f 2 >> k_inf.out
multi_agent | grep -P 'CI_flux' | cut -c 41-53 >> CI_flux.out

# ---------------
# POST-PROCESSING
# ---------------

# extract function value from the simulation output
#cut -c30-44 data > results.tmp
#awk '/1.880167/ {print $4}' data > results.temp
#awk ' NR % 19 == 0 {print}' results.temp > results.tmp
awk 'END {print} ' CI_flux.out >> results.tmp
# extract gradients from the simulation output (in this case will be
ignored
# by DAKOTA if not needed)
mv results.tmp $2
```