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DAKOTA DRIVEN OPTIMIZATION OF RESEARCH REACTOR OPERATION AND EXPERIMENTS: EXAMPLE OF NEUTRON ACTIVATION EXPERIMENTS

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ABSTRACT – Research reactors are commonly used for neutron activation analysis. A new neutron interaction simulation tool, PyNIC, has been developed for accurately predicting the dose rates and activities produced during neutron activation analysis at the University of Utah Nuclear Engineering Facility. To better enhance experiments and research conducted with the University's research reactor, optimization software, Dakota, has been coupled with PyNIC to optimize reactor operation when experiments are conducted involving neutron activation of the material samples. This novel approach is the first attempt at coupling neutron interaction simulation tools for research reactors with optimization software, in this case the Dakota software.

Introduction

The University of Utah Nuclear Engineering Program (UNEP) is home to the University of Utah TRIGA Reactor (UUTR) that was built in 1972 and has been operational since 1975. The UUTR has been used for a variety of research, testing and experiments throughout the years. Neutron activation analysis is a common non-destructive elemental concentration identification method and is heavily employed at the UUTR. As UNEP focuses on enhancing nuclear safety culture in a research reactor setting and education the need for accurately predicting the dose rates and activities generated from neutron activation analysis is needed [1-3]. The UNEP students developed a neutron interaction simulation tool, PyNIC to accurately predict the expected dose rates in neutron activation analysis at the UUTR [4].

The established nuclear safety culture at UNEP commands that the neutron activation analysis experiments are accurately predicted, planned and optimized. The whole process can be heavily automatized in coupling PyNIC with Dakota (Design Analysis Kit for Optimization and Terascale Applications) [5]. The Dakota (toolkit provides a flexible and extensible interface between simulation codes and iterative analysis methods. Dakota contains algorithms for optimization with gradient and nongradient-based methods such as PyNIC. The coupling of PyNIC with Dakota to optimize the design and performance of neutron activation analysis at the UUTR is presented in this paper. To the best of authors' knowledge, this is the very first coupling of the neutron activation analysis predicting calculations with Dakota for an optimized and highly efficient use of the reactor time and prediction of the best parameters needed for a neutron activation experiment.

1. UNEP's Nuclear Engineering Safety Culture

In 2009, as part of a re-vitalization of UNEP, it was noted that another improvement that could be made was to enhance the nuclear safety culture. A new unique safety culture platform was

established in 2012 and has become an integral part of every UNEP reactor operation, laboratory, exercise, research, training and experiments [6].

As part of a constant improvement process under the new safety culture, a more accurate and user – friendly neutron activation analysis prediction tool was developed to determine the dose rates and activity expected when irradiating materials in the UUTR. Being able to accurately predict the activity and dose rate of a sample after an irradiation is important so that the ideal irradiation parameters such as reactor power, irradiation time, irradiation location, decay time between irradiation and gamma spectroscopy, and gamma spectroscopy count time can be determined. It is also an important safety parameter to conservatively predict the expected dose rates from irradiating different material samples.

2 UNEP's Neutron Activation Analysis Predicition Tool - PyNIC

The UUTR has four different irradiation facilities that can be used for experiments and irradiations. They are located within the reactor core on different locations that provides different neutron flux and energy spectra properties and characteristics. Neutron activation analysis is usually performed by bringing the UUTR up to a specific power level between 1 kW to 90 kW which corresponds to a neutron flux of ~2.5×10^{12} n/cm^2·s. Once the specfiied power level is reached, the sample is placed into the indicated irradiation port (see Figure 1) for the pre-determined irradiation time. The sample is then removed from the UUTR where the dose rate measurement is taken at 1 foot away from the sample. Finally the sample is placed in a HPGe detector where counting of the activated samples are conducted. Therefore, the following parameters must be determined prior to neutron activiation analysis: Reactor power level, Irradiation port in the UUTR (Figure 1), Irradiation time of the sample within the port, Sample mass, Sample elemental composition, and Decay time between irradiation and counting.

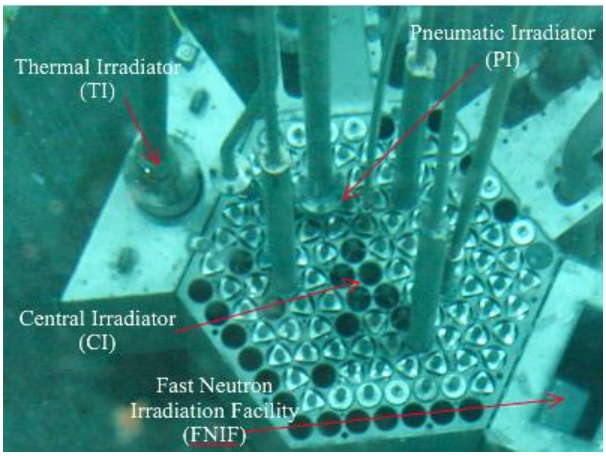


Figure 1: UUTR and Irradiation Ports

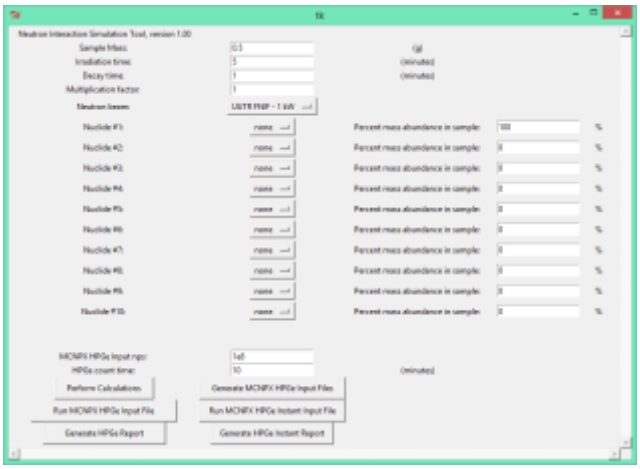


Figure 2: PyNIC Graphical User Interface (GUI)

In order to aid in the determination of the listed parameters, UNEP students and staff developed a new Python-based neutron interaction caculator (PyNIC) in 2014 [7]. Historically, the neutron activation analysis pre-calculators performed rough estimates of activation products usually only accounting for the thermal neutron flux of a neutron beam [8-11]. The PyNIC uses the entire neutron energy spectrum in order to achieve a higher level of accuracy in neutron activation

analysis and prompt gamma ray emissions from neutron capture and by calculating the activation across the entire neutron spectrum of the UUTR.

The PyNIC calculation is based on the neutron capture cross sections, selected inelastic scattering cross sections, and 23 selected fission cross sections in conjunction with the equations to calculate the activation products or immediate gamma emissions. The PyNIC also includes the ability for the user to perform an MCNP6 simulation of the gamma spectrum a user would expect to measure on the HPGe detector. A user – friendly graphical user interface (GUI) was developed so that a simple input of the above parameters is prompted when using PyNIC as shown in Figure 2. This all together has provided a unique tool for improved level of safety when irradiating materials in the UUTR.

3. Optimization of Neutron Activation Analysis Experiments at the UUTR with PyNIC and Dakota

Currently the only way for students or staff members to determine the best parameters for irradiating samples in the UUTR is to consecutively input varied parameters into the PyNIC tool. Although very unique and sysematic tool in prediciting the expeirments on neutron activation anlysis, this is time consuming. Therefore, an optimization tool is developed by coupling the PyNIC tool with the optimization software Dakota as sketched in Figure 3.

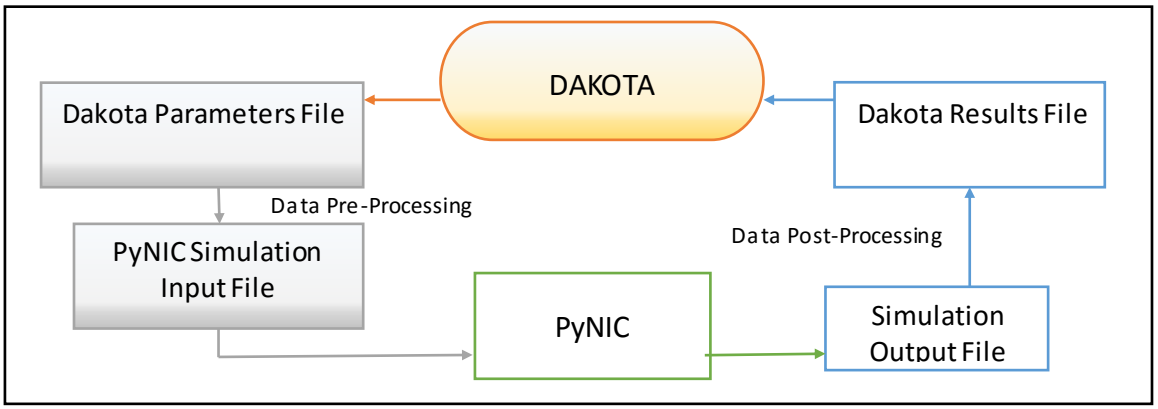


Figure 3: PyNIC and Dakota Flowchart

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 [5]. Sandia National Laboratories has released the Dakota software as open source and is thus readily available for use and implementation. A key Dakota advantage is access to a broad range of iterative capabilities through a single, relatively simple, interface between Dakota and the neutron interaction simulator. Trying a different iterative method or meta-algorithm typically requires changing only a few commands in the Dakota text input file and starting the new analysis. It does not require intimate knowledge of the underlying software package integrated in Dakota, with its unique command syntax and interfacing requirements. In addition, Dakota will manage concurrent executions of neturon interaction computational model in parallel, whether on a desktop or high-performance cluster computer. The coupling of these two codes results in determining the most efficient reactor power level, experimenation port, and irradiation time needed for various research and experiments being conducted at the UUTR in a safe and effective manner.

With the result of the coupling between Dakota and PyNIC a student or staff member can determine the best reactor power level, irradiation time, and irradiation port to conduct a given experiment the most effeciently and safely.

4. Conclusions

The coupling of an accurate neutron activation simulation tool, PyNIC, with optimization software, Dakota, has been investigated and discussed. This coupling will enhance the planning and predicition of irradiation expriments inclding safety and reliability of future research and experiments using the UUTR. Having the ability to quickly and accurately predict dose rates and activities of irradiation materials in research reactors will aid in many different future operations.

5. References

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