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Simulating Araponga - The High Resolution Diffractometer of Brazilian Multipurpose Reactor

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1. Introduction

The Brazilian Multipurpose Reactor (RMB) represents a milestone in the history of Brazilian science. Currently, RMB is the largest and most important drag project for the development of nuclear technology in the country, under the responsibility and coordination of the National Nuclear Energy Commission (CNEN). The main objectives of RMB and associated facilities are the production of radioisotopes and radiopharmaceuticals, aiming to meet the entire national demand of the Unified Health System (SUS) and the private network, irradiation and testing of nuclear fuels and structural materials, and the development of scientific and technological research using neutron beams [1, 2]. RMB will house the National Neutron Laboratory (LNN), the unit responsible for research activities with a suite of 17 instruments that manipulate neutron beams to investigate the structure of various materials [3]. Among the instruments that make up the LNN is the high-intensity neutron diffractometer, called the Flautim (scientific name = *Schiffornis virescens*). Beside the high-intensity diffractometer Flautim, Araponga will be on thermal guide one (TG1) of LNN. Powder diffraction is one of the most widely used techniques to study the structural and nanostructural properties of materials. The technique allows determination of long-range structure in polycrystalline materials, short-range atomic structure in disordered or amorphous materials, structural distortions, and any strain and crystal size induced changes to the structure [4]. Neutron powder diffraction has many attractive features, such as neutron penetrative ability, light element sensitivity, isotope dependent scattering, and its magnetic interaction [5]. Resolution and intensity are two essential characteristics of a powder diffraction instrument. While the resolution dictates the ability to discern the real space features of the material, the intensity dictates how quickly one can achieve such a measurement, and both are inversely related [6]. High intensity diffractometers require closer approximation to the neutron source, and therefore should be placed as close as possible to the reactor face. This is the first constraint that we must fulfill in simulations. Araponga is inspired by the Echidna instrument from the Australian reactor OPAL-ANSTO [7]. The basic configurations follow your model, but upgrades are necessary to meet the particularities of the RMB neutron beam. Monte Carlo simulations are indispensable tools in the design of nuclear facilities, from reactor cores to neutron scattering instruments. In this context, open source software McStas has been widely used to model neutron instruments and guides [8, 9]. The objective of this work is to simulate a simple configuration for Araponga, starting from the basic Echidna configurations. We determine the neutron flux at the sample location to ensure optimal values for data acquisition and discuss how improvements can be made in order to optical components that can optimize the diffraction technique.

2. Modeling Araponga

The linear dimensions of the neutron guides, as well as the relative distance to the reactor core and the components that make up Araponga can be found in Figure 1. It is important to note that the Araponga instrument is intended to be installed at the end of the TG1 thermal guide [3]. However, the input file to the McStas software contains data referring to the TG2 thermal guide. Therefore, in this work we will use this simplification as an initial approach to designing the instrument. We are certain that, soon, a complete study on Araponga will be able to be carried out with the input file referring to the TG1 thermal guide.

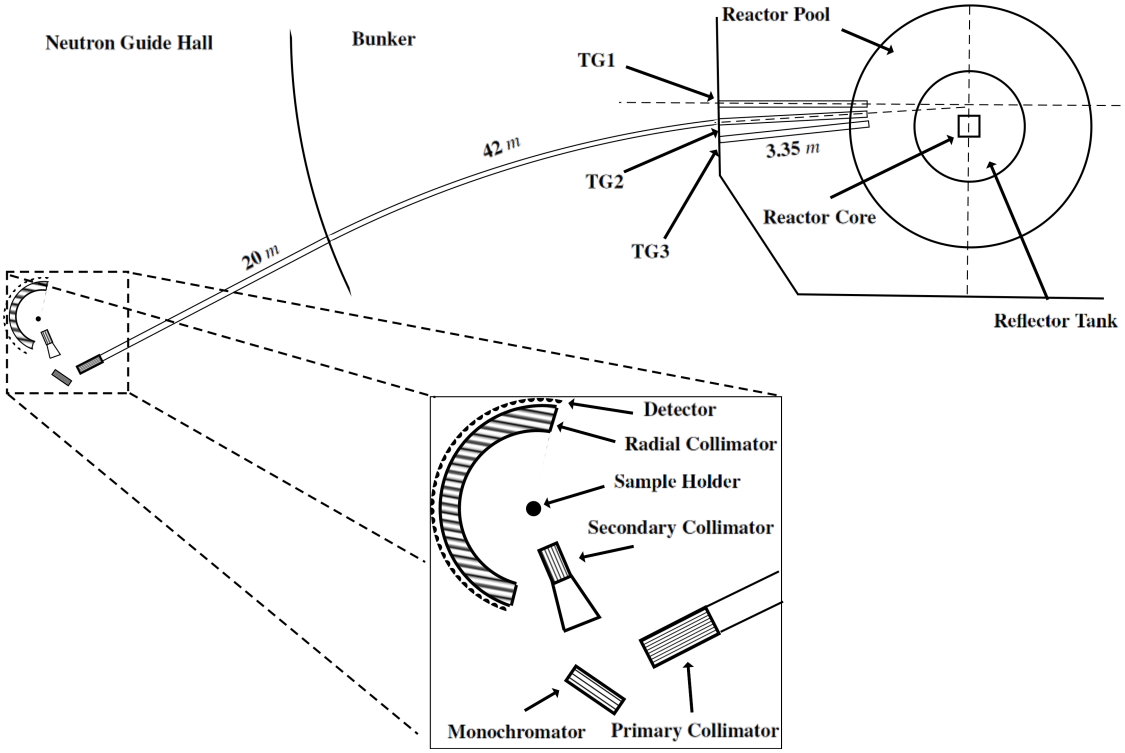

Figure 1: Scheme of the guide system from the reactor core to the Araponga instrument.

In this work, we use neutron guides in the bunker with three different curvature values, which were previously calculated to avoid the undesirable direct line of sight (LoS), that is, to ensure that each neutron undergoes at least one reflection on the guide wall [10]. The simulation parameters of each component of the diagram in Figure 1 are shown in Table I.

3. Results and Discussion

The results of the Monte Carlo simulations can be found in Table II. We can see that the flux at the Al_2O_3 sample site has excellent intensity, compatible with the best high-intensity neutron diffraction instruments located in international nuclear facilities [6, 7]. We observed that the maximum value was obtained for the configuration $R = 4410\ m$ and $d = 1.089$ Å. Although the results for flows, presented in Table I, show very small differences, we observed a tendency for guides with smaller curvature to present more reflections and consequently smaller flux values. Besides, considering that each monochromator d-spacing provides a different selected neutron wavelength. Therefore, one can only compare flux values of the same monochromator. In this

Table I: Components and parameters of McStas simulations.

Components	**Parameters and characteristics**
In-Pile Guide	Section (width x height) = 5 cm x 30 cm; Length = 3.35 m; Curvature = infinity (straight guide); Supermirror index $M = 3$ (all sides);
Bunker Guide	Section (width x height) = 5 cm x 30 cm; Length = 3.35 m; Curvatures = 4410 m, 4745 m, 5080 m; Supermirror indexes: $M_{out} = 3$, $M_{top} = 3$, $M_{bottom} = 3$, $M_{in} = 2.5$;
Hall Guide	Section (width x height) = 5 cm x 30 cm; Length = 20 m; Curvature = infinity (straight guide); Supermirror index $M = 2.5$ (all sides);
Primary Collimator	Section (width x height) = 5 cm x 30 cm; Length = 0.7 m; Divergence = 10’;
Monochromator	Section (width x height) = 5 cm x 30 cm; Germanium Monochromator = Vertical Focusing; Crystallographic planes: 0.863 Å (533), 1.089 Å (511), 1.714 Å (311); Take-off angle = 45 degrees;
Funnel Guide	Input Section (width x height) = 5 cm x 30 cm; Output Section (width x height) = 5 cm x 13 cm; Length = 1.8 m; Supermirror index $M = 2.5$ (all sides);
Secondary Collimator	Section (width x height) = 5 cm x 13 cm; Length = 0.3 m; Divergence = 10’;
Sample	Cylindrical-V 4 cm high, inner radius 0.25 cm and outer radius 0.30 cm; Al_2O_3 powder sample;

sense, it is possible to observe that the curvature value growth imposes higher flux values, except for curvature 5080 m - 1.089 Å case.

Since guide curvatures determine different wavelength neutron transport efficiency and output flux divergence, a direct correspondence between flux values and curvature is not always possible. From that matter, it is important to point out that fine adjustments in the primary and secondary collimators can bring optimal conditions for the diffraction technique. All these aspects are also directly related to the flux spectra that reaches the instrument primary collimator.

4. Conclusions

The simulation results for the neutron flux at the sample site are extremely encouraging. We started with a basic configuration for the Araponga instrument and many adjustments could be made to optimize the neutron diffraction technique. The results obtained are compatible with state-of-the-art instruments from international installations [6, 7]. Our model will receive new attributes after the simulations for the TG1 thermal guide, where the high intensity neutron diffractometer, called Flautim, will be localized [3]. The optimization problem has many variables, such as the choice of collimators and evaluation of beam divergences in curved sections. Soon, we will present more complete discussions about the wavelength ranges for each studied configuration.

Table II: Monte Carlo simulation results for neutron flux at the sample location for parameter sets. The *hkl* lattice parameters are the Miller indices.

R (m)	d (Å) (hkl)	λ (Å)	Flux (n/cm^2s)
4410	0.863 (533)	1.22	1.072×10^6
	1.089 (511)	1.54	1.130×10^7
	1.714 (311)	2.42	4.860×10^6
4745	0.863 (533)	1.22	4.158×10^6
	1.089 (511)	1.54	3.685×10^6
	1.714 (311)	2.42	2.761×10^6
5080	0.863 (533)	1.22	3.041×10^6
	1.089 (511)	1.54	5.114×10^6
	1.714 (311)	2.42	2.478×10^6

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