

# NEUTRON DIFFRACTOMETRY CHANNEL OPTIMIZATION TO OBTAIN THE HIGHEST NEUTRON FLUX AND THE LEAST FAST NEUTRON NOISE

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## Abstract

Neutron powder diffraction (NPD) is complementary to many other materials characterization techniques. Some material analyses are not possible using the other procedures such as investigation of magnetic properties of materials or distinguishing between the adjacent elements in the periodic table. In overall, neutron diffraction could involve many unique advantages: the neutron scattering strength is not dependent on the atomic number. In the present work, NPD system of 5 MW Tehran Research Reactor was modeled using MCNPX2.6.0 and Vitess 3.3a codes in details. The system uses a PG reflector to reflect 0.02–0.33 eV neutrons through the second collimator. The neutron spectra achieved by Vitess 3.3a code at sample position was compared with the available experimental data. Impact of Al<sub>2</sub>O<sub>3</sub> filter on fast neutron noise at the sample position was investigated. The obtained data from the simulations showed good conformity with the experimental measurements. Our simulations showed registration of an adequate thickness of Al<sub>2</sub>O<sub>3</sub> inside the NPD facility could decrease the fast neutron noise drastically.

**Keywords:** Tehran research reactor, neutron powder diffraction, MCNPX2.6.0, Vitess 3.3a

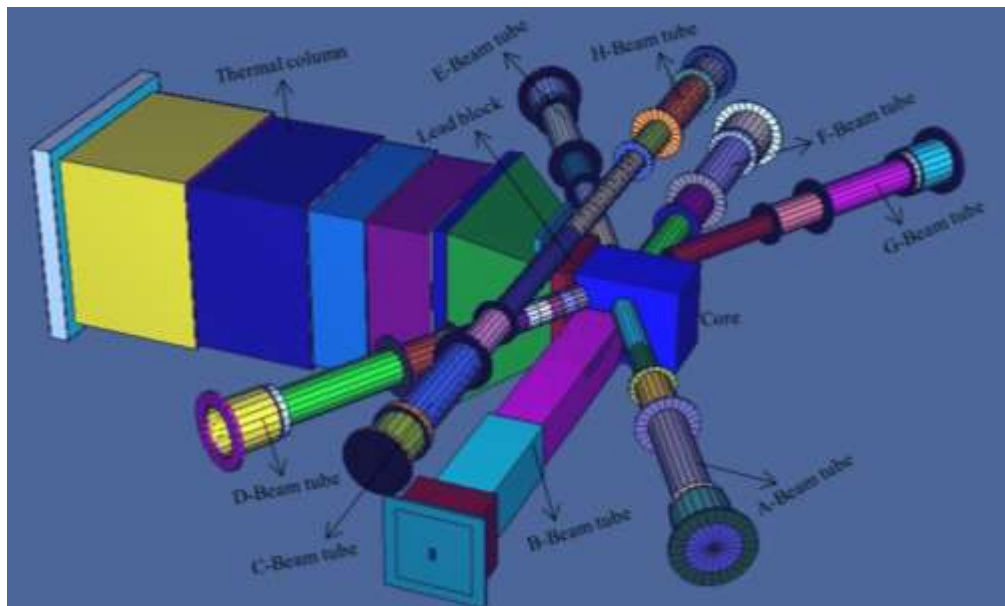
## Introduction

Whereas the large capital costs associated with intense neutron sources, neutron diffraction is rarely the first technique used to study a particular material or a highly specialized way to provide critical information or facilitate a critical in situ experiment. It is possible to observe the effect of light elements in the presence in heavy ones in neutron diffraction patterns. Neutrons are deeply penetrating so they can diffract off specimens contained in cryo-refrigerators or furnaces, making it easy to examine materials under special conditions and in special environments. Unlike the case for X-Rays, the scattering of neutrons from materials can be accurately calculated making comparison to theoretical [1]. Today neutron diffraction plays a vital role in vast domains of science and technology while it makes ability of observation and analysis of many materials which was not possible by XRD or other diffraction techniques.

Mazzochi et al. reported a powder diffractometer has been recently installed on the IEA-R1 reactor at IPEN-CNEN/SP. IEA-R1 is a light-water open-pool research reactor. At present it operates at 4.5 MW thermal with the possible maximum power of 5 MW. At 4.5 MW the in-core flux is ca.  $7 \times 10^{13} \text{ cm}^{-2}\text{s}^{-1}$ . In spite of this low flux, installation of both a position-sensitive detector (PSD) and a double-bent silicon monochromator has turned possible to design the new instrument as a high-resolution powder diffractometer [2].

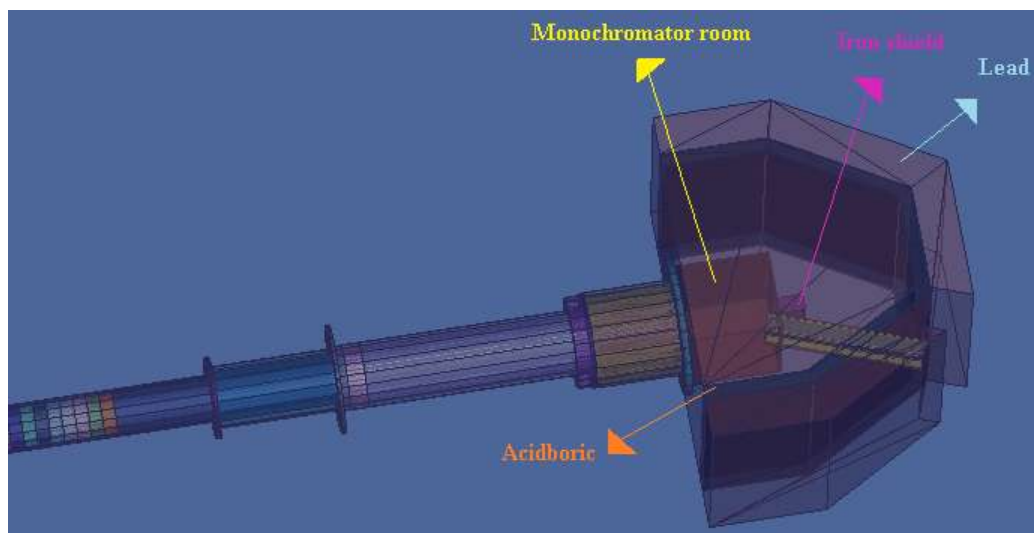
## Material and methods

TRR is a 5 MW pool-type light water research reactor. Its fuel assemblies contain low enriched uranium fuel plates in the form of  $U_3O_8Al$  alloy. The users apply two sections of the reactor pool. One of the sections contains experimental facilities like beam tubes, rabbit system, and thermal column. The other section is an open area for bulk irradiation studies. Fig. 1 shows the schematic view of TRR pools and irradiation facilities. TRR was simulated in details using MCNPX 2.6.0[3] code as shown in Fig.1.



**Fig. 1.** Position of different beam lines of TRR modeled by MCNPX 2.6.0

In this facility D channel was allocated to NPD system. The equipped D channel was modeled using the Monte Carlo-based computation code (Fig.2).



**Fig. 2.** D channel arrangement of NPD facility of TRR

Neutron and photon flux distributions were calculated along the NPD channel using the computational code. In addition, neutron spectra at the beginning of the NPD channel obtained from the MCNPX2.6.0 code was introduced as an input source for the Vites 3.3a code [4] to investigate the reflected neutron spectra from the NPD system monochromator.

The PG monochromator is used in the current NPD facility of TRR was introduced in the Vites 3.3a code according to Table 1.

**Table 1-** PG monochromator characteristics

d-spread	PG(002): $0.2 - 2' 10^{-3}$
d-spacing	PG(002): 3.332 Å
Thickness, width, height	0.2, 7.5, 5
Mosaic factor	2
d range factor	3

In pyrolytic graphite the crystallites are aligned to a high degree with their hexagonal c-axes parallel, whereas the a-axes are oriented at random. Therefore, the reflected neutrons are from the (00l) planes satisfying the Bragg equation:

$$n\lambda = 2d_{hkl}\sin\theta_{00l} \quad (1)$$

Where,  $n$  is the order of reflection,  $\theta_{00l}$  is the glancing angle to the (00l) plane [5].

Neutron flux on wavelength was calculated after the PG monochromator and at the sample position, which is located 100 cm far from the second collimator exit.

The code uses F4 tally card to calculate neutron flux via the following equation [6]:

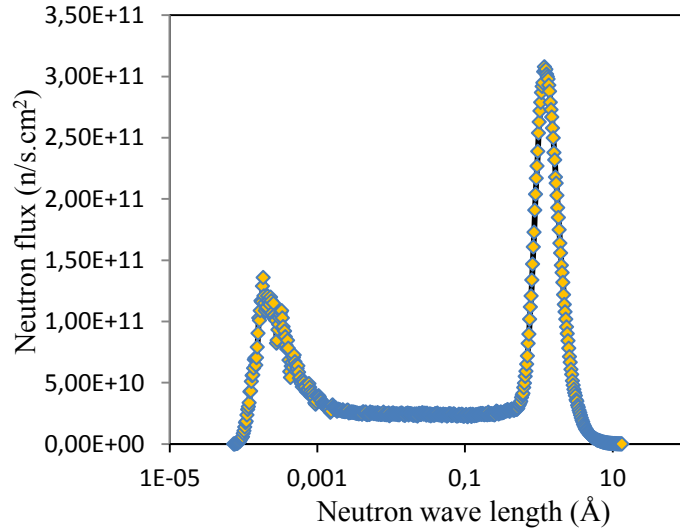
$$F4 = \frac{1}{V} \int_V dV \int_E dE \int_{4\pi} d\Omega \Phi(r, E, \Omega) \left( \frac{\#}{\frac{cm^2}{source\ particle}} \right) \quad (2)$$

Neutron noise was determined in the pathway of the neutrons flying directly from the second collimator to the sample position. The calculated neutron flux at the sample position was compared with the experimental data.

Al<sub>2</sub>O<sub>3</sub> filter application inside the NPD facility was investigated to decrease the fast neutron noise at the sample position.

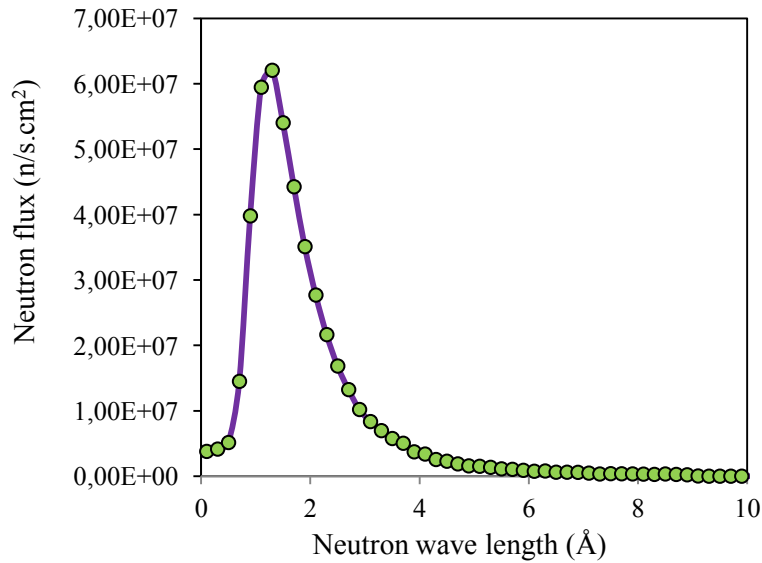
## Result and discussion

D channel of the 5 MW reactor has a 305 cm length, at the final section of the channel a collimator was placed. The first collimator is a rectangular Soller-type collimator made of steel with the dimension of 6×11×120 cm. Neutron spectra was calculated using MCNPX2.6.0 at the beginning of the D channel (Fig.3).



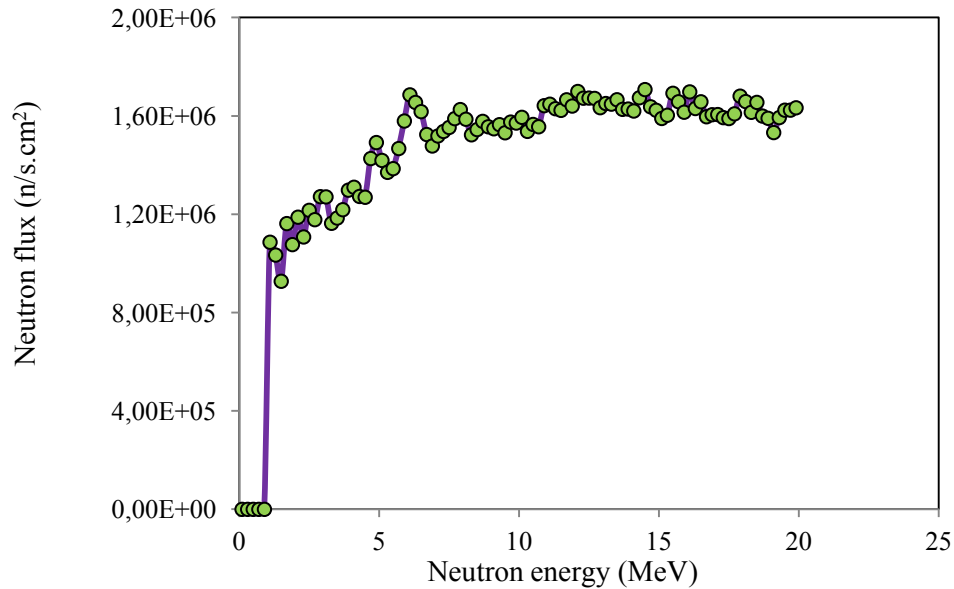
**Fig. 3.** Neutron spectra on wavelength at the beginning of NPD D channel facility of TRR

As the figure shows, there is a thermal neutron flux in order of  $10^{11}$  n/s·cm<sup>2</sup> at the beginning of D channel. The obtained spectra from the MCNPX2.6.0 code exported to Vites 3.3a code and the departing neutrons from the first collimator were investigated. According to Fig.4, the thermal neutron intensity drops  $10^3$  orders during its flight along the 3-meter D channel and its equipped collimator.



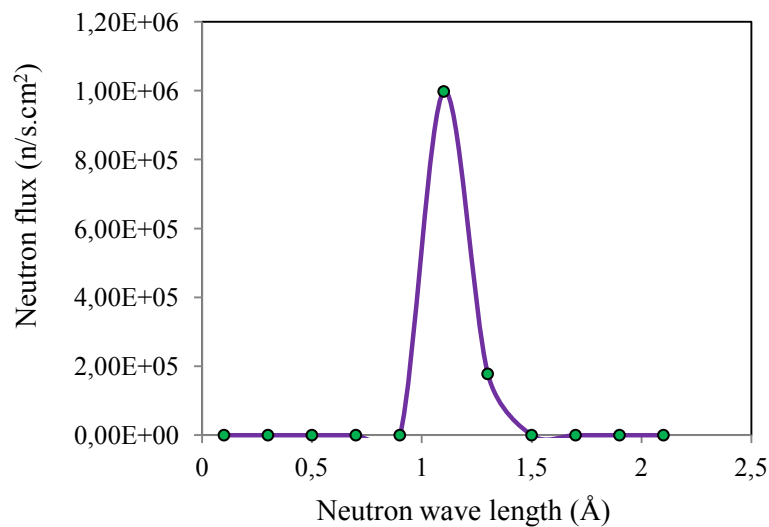
**Fig. 4.** Neutron spectra on wavelength at the exit of first collimator

Also fast neutrons with an intensity in order of  $10^6$  n/s·cm<sup>2</sup> are exiting from the first collimator toward the PG monocromator of the NPD system (Fig.5).



**Fig. 5.** Neutron spectra on energy at the exit of first collimator

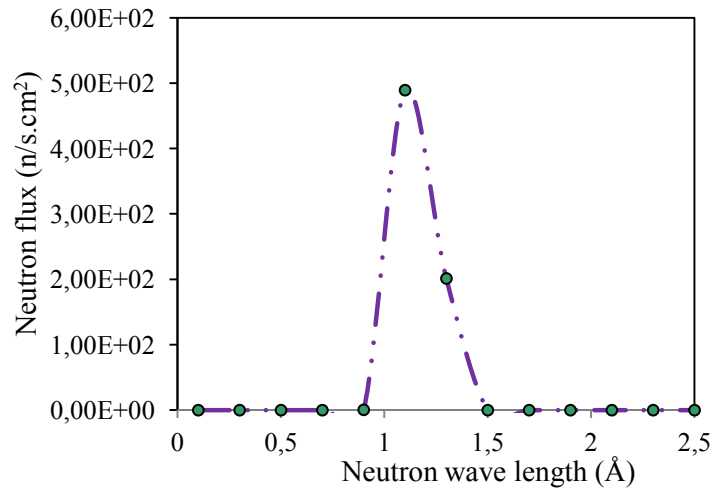
The collimated neutrons collide on the PG monochromator positioned 15 cm far from the first collimator exit. The channel arrangement simulation by Vites3.3a code showed the reflected neutrons from the monochromator would have a peak intensity of  $1 \times 10^6$  n/s·cm<sup>2</sup>. The monochromatic neutrons have 1–1.5 Å wavelength (Fig.6).



**Fig. 6.** Neutron flux intensity on wavelength after monochromator reflection

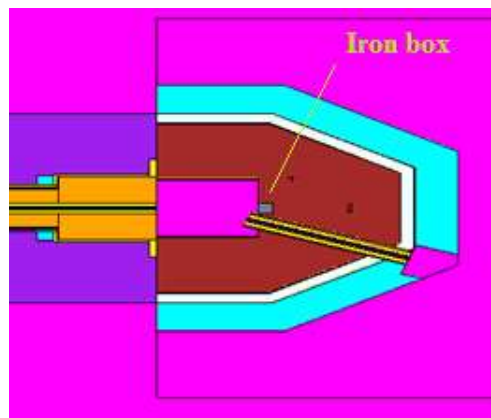
After reflection of low-energy neutrons (1–1.5 Å), the other neutrons available in the incident neutron spectra pass through the monochromator and follow their track approximately directly. Hence, as the Vites code calculations show there is not fast neutron noise in the second collimator track. As illustrated before, a 60 cm long soller-type collimator was placed in the pathway of neutrons. The sample Table was placed at 122 cm interval than the second collimator exit. Vites 3.3a code calculations showed the thermal neutron flux intensity at the

sample position is  $0.5 \times 10^3 \text{ n/s}\cdot\text{cm}^2$  which has 40.5% relative discrepancy than the measured value;  $0.84 \times 10^3$  (Fig.7).

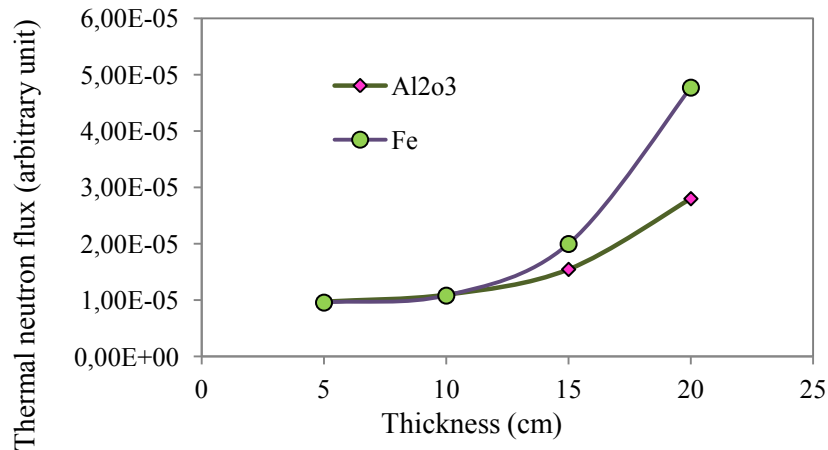


**Fig. 7.** Neutron flux intensity on wavelength at the sample position (122 cm from the second collimator)

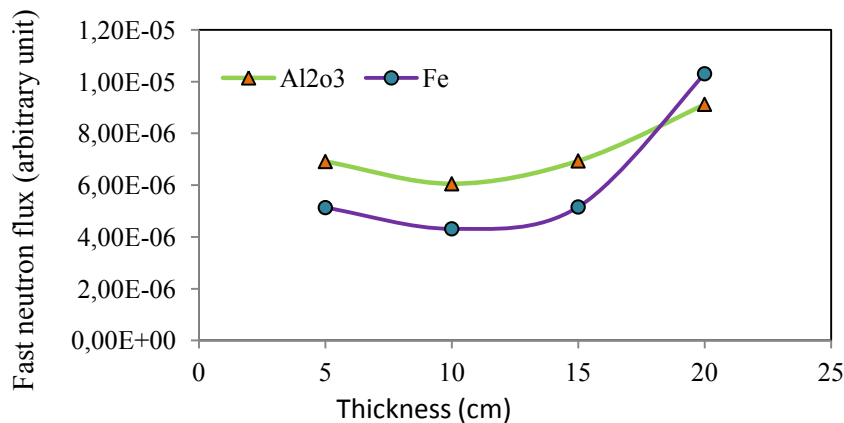
Paraffin was filled around the monochromator room and an iron box with  $10 \times 10 \times 10 \text{ cm}^3$  (Fig. 8) was placed in the fast neutron pathway, the results showed higher thickness causes the fast neutron enhancement (Fig.9,10). The optimized dimension decreases the fast neutron flux up 36%.  $\text{Al}_2\text{O}_3$  was investigated also but the obtained results showed the material positioning at this place is not effective than the iron box. Application of  $\text{Al}_2\text{O}_3$  at the beginning of the channel resulted in 55% reduction of fast neutrons. Another iron box application after the shielding of monochromator room resulted in 66% reduction of the leaked fast neutrons. Application of  $\text{Al}_2\text{O}_3$  after the monochromator room was not as efficient as iron box because it causes only 17% reduction of the fast neutrons.



**Fig. 8.** Iron box view after monochromator room



**Fig. 9.** Thermal neutron flux variation on filter thickness



**Fig. 10.** Fast neutron flux variation on filter thickness

## Conclusion

Vitess code application could desirably estimate the different structures of the system. This study showed Al<sub>2</sub>O<sub>3</sub> and Fe application in different parts of the system can decrease the fast neutron flux considerably.

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