

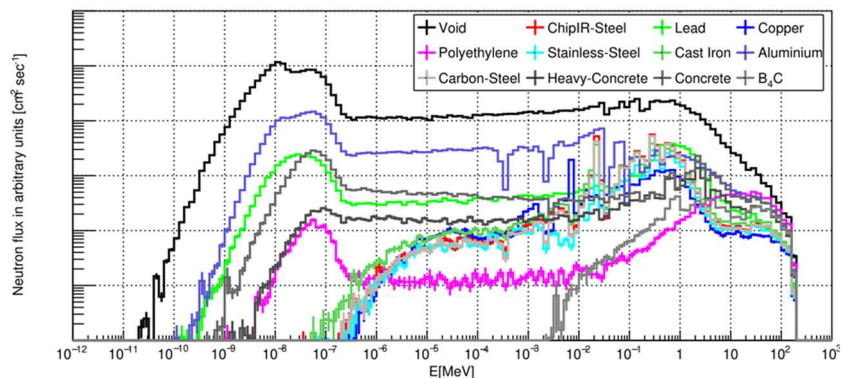
VESPA project: brief report on the activities done between mid-October 2021 and late April 2022

The present document is a brief report dealing with the activities of the VESPA team performed in the period between mid-October 2021 and late April 2022, *i.e.*, from the previous Spectroscopy STAP meeting (on the 15th/10/2021) until now. We will focus on the three following points, including a detailed answer to the remarks contained in the latest report by the ESS Spectroscopy STAP panel:

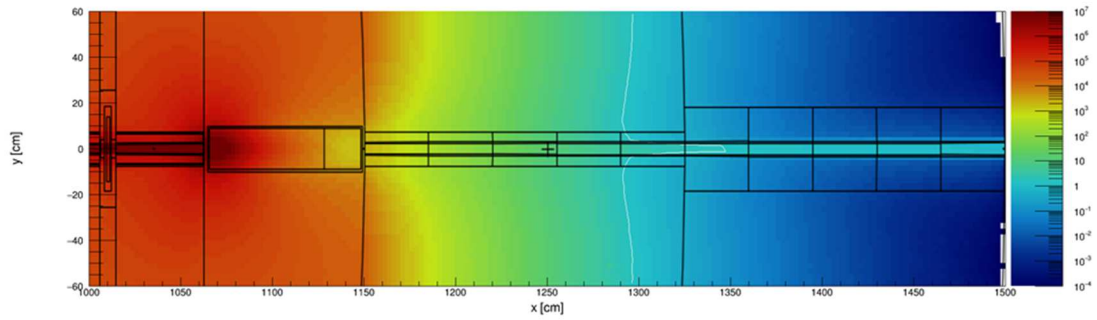
- 1) Advances in the design of the VESPA “heavy shutter”.
- 2) Update on the performance simulations of the VESPA beamline and the instrumental software for ‘day 1’.
- 3) Reply to the latest report of the ESS Spectroscopy STAP panel.

1) Advances in the design of the VESPA “heavy shutter”

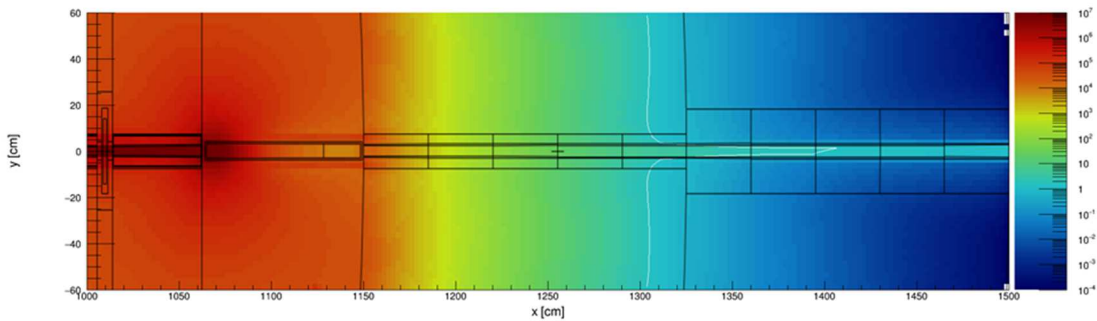
The preliminary design for the so-called VESPA “heavy shutter”, which is currently under investigation, consists in two main bulk materials: copper and B₄C. These materials were chosen to be studied by a set of MCNP simulations in which a neutron beam with a known spectrum impinges on a parallelepiped (25 cm thick), made of a single material among those listed in the legend of the following plot:



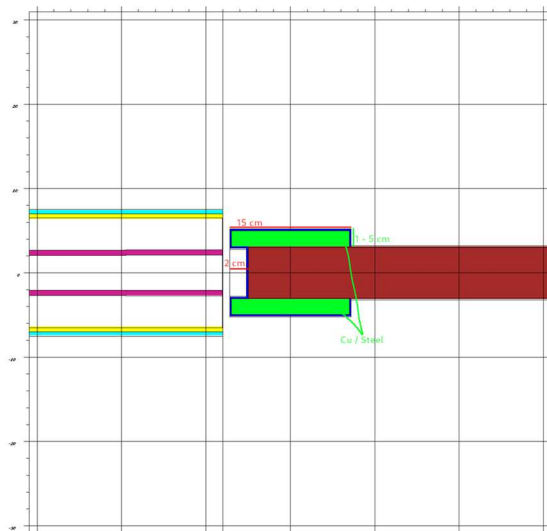
The curves above show several neutron spectra calculated after these bulk materials. “Void” shows the initial neutron spectrum of the beam. According to these results, the “heavy shutter” was designed as a parallelepiped made of two main materials: a block of copper followed by a 20 cm-thick B₄C block. The base of such parallelepiped is a square whose side is 20 cm long. In order to determine the thickness of the copper block, a set of MCNP simulations was performed. In each simulation this block had a different thickness: 48, 50, 51, 52, 53, 58, and 63 cm. The last has proven to match the requirements to not exceed 2.5 μSv/h at the exit of ESS bunker wall feed-through, as shown in the following neutron dose rate map (where the white line is an isodose line set at 2.5 μSv/h):



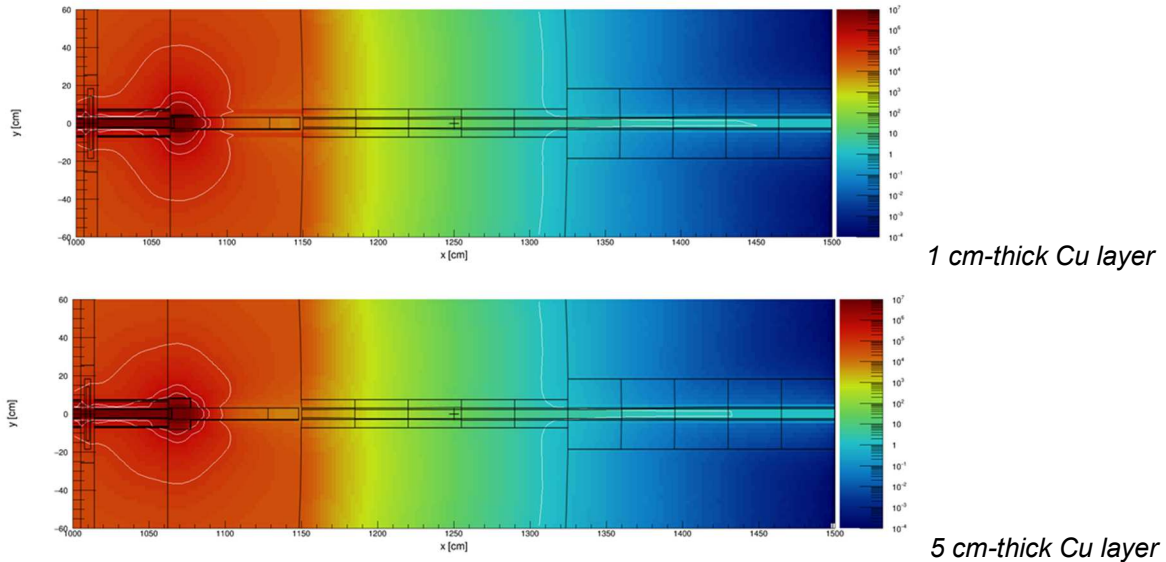
The side length of the parallelepiped's base was determined by a set of MCNP simulations in which such a dimension was varied from 20 to 8 cm, in steps of 2 cm each. The results show that the thinnest design, with a basis of 8 cm×8 cm still meets the requirements, as proven by the neutron dose rate map for such design given below:



The currently proposed design for the “heavy shutter”, according to these investigations, consists in a copper block of 63 cm followed by a B₄C block of 20 cm, enclosed in a steel envelope which is 2 mm thick. These two blocks, placed one after the other, form a parallelepiped of 83 cm, with a squared base of 8 cm×8 cm. Currently, a shroud for the “heavy shutter” is under investigation. It would help reducing the scattered radiation which leaks from the beamline and could affect neighbouring instruments. That shroud would consist in some layers of stopping materials. Considering that the previous results show a hotspot in the neutron dose rate in the region where the neutron beam impinges on the “heavy shutter”, a preliminary set of MCNP simulations was performed, where an extra layer of material was added to that region. Two different materials were investigated: copper and steel. The investigated geometry is shown in the following picture:



The geometric parameter in green is the one that was varied from 1 to 5 cm, in steps of 1 cm. The results show no relevant difference in the neutron dose rate maps for steel and copper, while it is still under evaluation the impact of a different thickness for this extra layer. As representatives, the neutron dose rate maps for a 1 cm-thick layer of copper and a 5 cm-thick layer of copper are given below:



The four whitish isodose lines are set at 1.5, 1×10^5 , 5×10^5 , and 1×10^6 $\mu\text{Sv/h}$. They show that a different thickness value affects the shape of the dose rate distribution around the neutron hotspot, but does not significantly reduce it. Further analysis are needed in order to improve the design of the shroud so to minimize the leaking radiation.

2) Update on the performance simulations of the VESPA beamline and the instrumental software for 'day 1'

The simulation of the instrument performances is an essential tool for an effective design of the main neutron components, from their conceptualization to the production of a detailed model. The VESPA team has been using two Monte Carlo simulation packages, i.e., *McStas* and *MCNP*, to address neutronic calculations regarding the *beam transport and conditioning system* (BTCS) and the *scattering characterization system* (SCS) on one side, and the biological/background shielding on the other, respectively. The update on the shielding calculations has been already reported in paragraph (1) of the present document.

As for the main components of the primary spectrometer, i.e., the guide and chopper systems, their design is currently "frozen", waiting for the start of tender for the former item, which will be outsourced, and for the begin of the engineering design for the latter, which will be procured within the *ESS Chopper Common Project* (CCP). In the case of the primary spectrometer, the simulative efforts needed to produce the current model have been addressed to maximize the flux at sample position and the energy resolution in the so-called *finger-print region* (i.e., 60-220 meV), that is particularly meaningful in chemico-physical applications (see Figure 1).

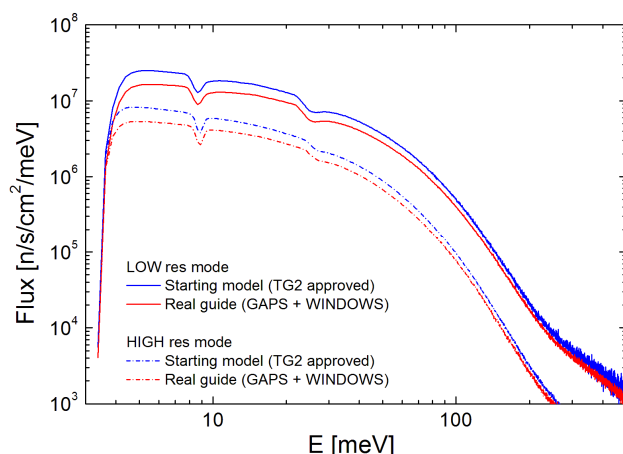


Figure 1. Flux at sample position for both the conceptual model, as approved at TG2 (blue curves), and a more detailed model including guide segmentation, interruptions, and windows (red curves).

As for the secondary spectrometer (and diffractometer), the *McStas* simulation package has allowed to efficiently drive their conceptual design. At the current stage of the project, this Monte Carlo tool is also used for the refinement of some specific components. In particular, through a customized “delta-comb” sample, we have calculated the relative energy resolution for different degrees of mosaicity of the HOPG analyzers (see Figure 2, left panel), while the extension of the detector surface and the elastic line access have been optimized by using a vanadium-like scatterer. Also for the evaluation of the diffraction capabilities, we have used a customized comb of Bragg reflections with no intrinsic line broadening and extracted the relative d -spacing resolution (Figure 2, right panel) for the different parameters that we need to optimize.

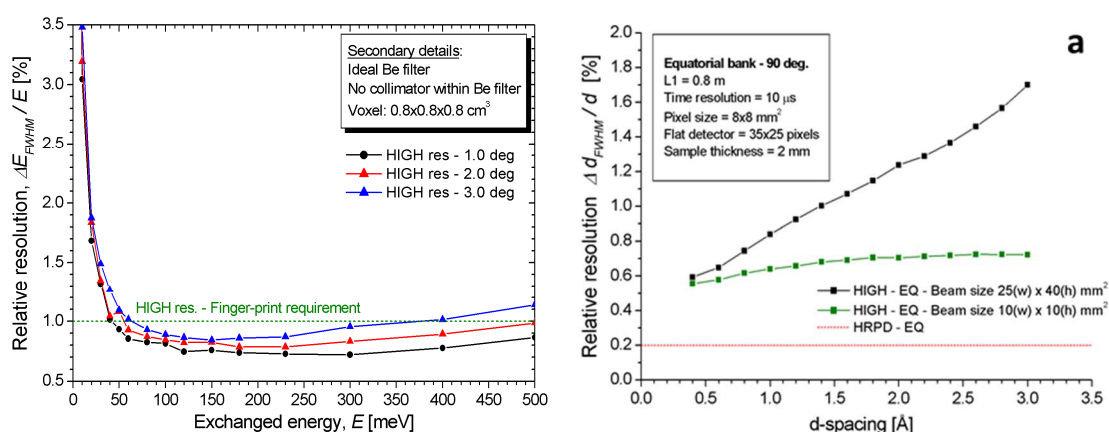


Figure 2. (Left panel) relative energy resolution of the spectrometer at different degrees of analyzers mosaicity. (Right panel) relative d -spacing resolution of the equatorial diffraction bank with a full beam size ($25 \times 40 \text{ mm}^2$) and a reduced beam size ($10 \times 10 \text{ mm}^2$).

In any case, the detailed design of the main components of the secondary spectrometer is currently in progress and needs to be furtherly integrated with ancillary equipment, e.g., sample environment equipment, vacuum tank, Be-filter cold-heads, detector back-end electronics, mounting frames. In

this perspective, the hiring of additional scientific and engineering staff, fully devoted to the development of this part of the instrument, is particularly urgent for the VESPA project.

VESPA has been designed to be a neutron instrument fully dedicated to vibrational spectroscopy. This means that VESPA's main topic will be the study of undispersed (or weakly dispersed) excitations in low-temperature solid powders. In addition, since the majority of the samples are largely protonated, the neutron signals measured by VESPA will be largely incoherent. Putting these two things together it turns out that, differently from the standard time-of-flight and triple-axis neutron spectrometers, instruments like VESPA will pay relatively little attention to the momentum transfer, $\hbar\mathbf{Q}$, focusing on the energy transfer, $\hbar\omega$, *i.e.*, on its range (0-500 meV) and its relative resolution (0.9-2.8%). This choice does not imply that $|\mathbf{Q}|=Q$ does not play an important role in shaping the recorded neutron spectra (quite the opposite: it is crucial to determine the intensity, but not the frequency, of the observed excitations). However, Q turns out to be a single-valued, monotonic function of ω , weakly dependent on the scattering angle θ , so that: $Q=Q(\omega,\theta)$. In other words, instead of exploring a large area of the kinematic plane (ω,Q) , instruments like VESPA probe narrow curved stripes on this plane, where, for ω large enough, $Q \propto \omega^{1/2}$. So, even in presence of large differences in θ (say, backscattering θ_B versus forward-scattering θ_F), the discrepancy between $Q(\omega,\theta_B)$ and $Q(\omega,\theta_F)$ would turn out to be rather modest (but not negligible). Finally, it is worth mentioning that on VESPA all the detector tubes will be arranged in a circular way in few detector blocks exhibiting (plus or minus a few degrees) equal values of θ_n (*e.g.*, two values on VESPA), obviously corresponding to the same number of $Q_n=Q(\omega,\theta_n)$ stripes ($n=1,2$). Given the aforementioned scenario, it will be natural on instruments like VESPA to have very simple data reduction routines, transforming the *time-of-flight* (t) neutron counts of an individual tube j , $C_j(t,\theta_j)$ (belonging to the n^{th} detector block) into the corresponding *generalized scattering law* $\Sigma_j(\omega,Q_n)$. This is very standard on inverted-geometry spectrometers and so we are not going to discuss this point. The only issue which is important to point out is that, due to the detector block structure, all the $\Sigma_j(\omega,Q_n)$ signals exhibiting the same n , are actually almost identical (in terms of ω , Q and energy resolution), except for a constant scaling factor due to small solid angle differences. So on VESPA all these signals can be safely summed together giving rise to four functions $\Sigma(\omega,Q_n(\omega))$, which are simple three-columns histograms: $\hbar\omega$, Σ , $\delta\Sigma$ (*i.e.* energy, generalized scattering law, and its uncertainty), since Q_n is now a monotonic function of ω , easy to be determined. In conclusion, independently of the number of detector tubes, VESPA's data size, after performing a preliminary data reduction procedure, will be always extremely small. Although the large majority of neutron vibrational spectroscopists perform no further data analysis, since they usually deal with $\Sigma(\omega,Q_n(\omega))$ in the same qualitative way as it is currently done with Raman and infrared spectra, it is in principle possible to set up a series of advanced data analysis routines going through the standard steps common to all inelastic neutron scattering measurements: (a) sample cell signal and fast neutron background subtraction; (b) sample self-shielding correction; (c) multiple scattering evaluation and removal; (d) heavy nuclei scattering evaluation and removal (only for simple systems); (e) multiphonon contribution evaluation and removal (only for simple systems).

As we have already pointed out, in this kind of spectroscopy neutron data manipulation is reduced to a minimum. On the other hand, it is considered very important to produce simulated neutron vibrational spectra starting from the outputs of various DFT codes (*i.e.*, VASP, CASTEP, ABINIT, QUANTUM_ESPRESSO etc.). In other words, while from the vibrational eigenvalues and eigenvectors calculated by these programs it is straightforward to estimate the so-called k atom-projected density of phonon states, $G_k(\omega)$, it is much more demanding to evaluate $\Sigma(\omega,Q_n)$, since various effects have to be taken into account: (i) sum over all the non-equivalent atomic species (labeled by k) contained in the sample; (ii) calculation of a number (at least 6) of overtones and combinations, including a folding with the low-energy lattice modes (the so-called "phonon wings");

(iii) calculation of anisotropic spectroscopic effects and, subsequently, of spherical powder averages;
(iv) inclusion of possible coherence effects; (v) instrumental energy resolution broadening.
At the moment, the best programs able to perform most of these tasks are surely OCLIMAX (by Oak Ridge National Laboratory, USA) and AbINS (by Rutherford Appleton Laboratory, UK), which, for this reason, have to be considered as the benchmark codes in this spectroscopic area.

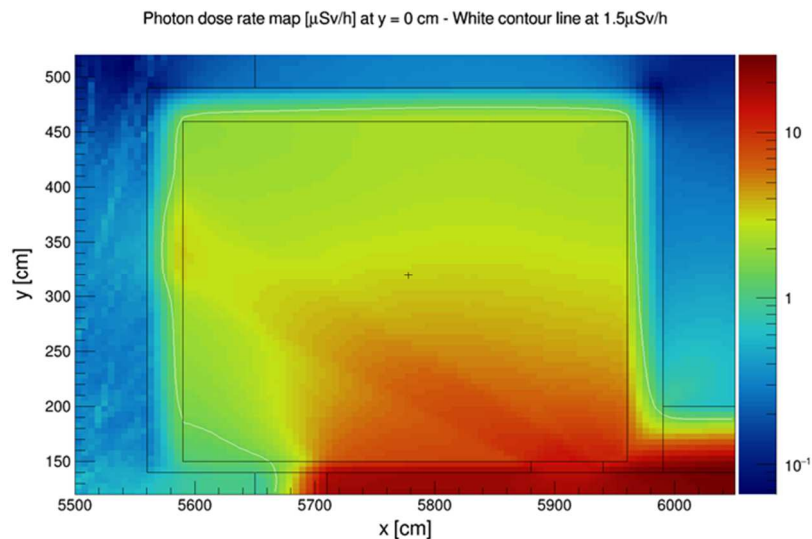
3) Reply to the latest report of the ESS Spectroscopy STAP panel

Concerning VESPA, the following recommendations were contained in the mentioned report from the ESS Spectroscopy STAP panel:

“(...). Shielding calculations for the cave have been completed, showing that 60 cm walls will be required (in some parts). Figure 2 reports neutron doses but we believe it is quite important to check gamma doses as well – has this been done?”

“(...). The impact of the HOPG mosaic spread was further analysed in detailed McStas calculations, but the team doesn't reach a final conclusion/recommendation.”

The former question has been positively answered as shown in the following example of the photon (gamma rays) dose rate map for the upper part of the VESPA cave:



The latter question has been dealt with the first part of paragraph (2) and the final conclusion is the following: 1.5 deg. of HOPG mosaic spread.

The VESPA Team