2nd Oct. 2020

Spectroscopy STAP meeting (19th-21st October 2020)
VESPA spectrometer: brief report on the activities between April and September 2020

The present document is a brief report dealing with the activities of the VESPA team performed in the period between the end of April 2020 and mid-September 2020, i.e. essentially from the previous Spectroscopy STAP meeting until now. In this period, various European countries experienced a complete lockdown for several weeks due to the Covid-19 pandemic disease. Consequently, all the Italian research institutes and universities were partially shut, forcing their staff to work from home when possible (the so-called “smart work”). In our case, the impact we faced was mainly due to the lack of access to resources, as CNR institutes and university departments were formally closed. However, we experienced only minor delays in the team activity because, at the present stage of the project, most of the scientific and engineering tasks could be performed from remote, as well as the preliminary contacts with possible suppliers.

Leaving aside the detailed managerial aspects of the VESPA team’s work (which could be hardly summarized here), we will focus on the following points:
1) Work on Highly Oriented Pyrolytic Graphite (HOPG) crystal analyzers.
2) Document *“H1 and H2 scenarios for the radiation shielding of VESPA”*.
3) VESPA instrument design and procurement: the overall project status.

1) Work on HOPG crystal analyzers

We have started considering the various options for the HOPG crystal analyzers offered by PANASONIC, with which an informal contact had been established in the past. At the present stage of the design, our attention has been focused on the crystal mosaicity choice, a crucial parameter strongly influencing not only the resolution performance of the secondary spectrometer (i.e. from sample to detectors), but also its cost. Preliminary simulations, performed after the TG2 approval (in summer 2018), suggested that a mosaicity-value of 4° should be considered as an upper limit, even though HOPG with such a value is currently under development by PANASONIC. Now, the available mosaicity options for the PANASONIC HOPG crystals are those listed in Tab. I.

Product name	*Estimated mosaicity* [degree]
PANASONIC PGCX07	0.8 ± 0.2
PANASONIC PGCX10	1.5 ± 0.5
PANASONIC PGCX20	2.5 ± 0.5

Tab. I. Mosaicity estimates for the HOPG crystals by PANASONIC.

Since we are interested to determine the reduction of the resolution performance as a function of the HOPG analyzer mosaicity, we have performed accurate *McStas* simulations in the VESPA High-Resolution (HR) mode using an ideal inelastic sample consisting in a comb of delta-function bands placed in the so-called “fingerprint” energy transfer range (i.e. 60-220 meV) and also above it (i.e. 300-500 meV). Results are reported in Fig. 1, where the relative energy resolution is plotted as a function of the mosaicity for the different energy transfers considered. As it appears evident, the high-level scientific requirement of 1% for the relative energy resolution is fulfilled for all the mosaicity options in the “fingerprint” region, while at higher energy transfers (i.e. 300-500 meV) the 2° option clearly represents the upper limit.

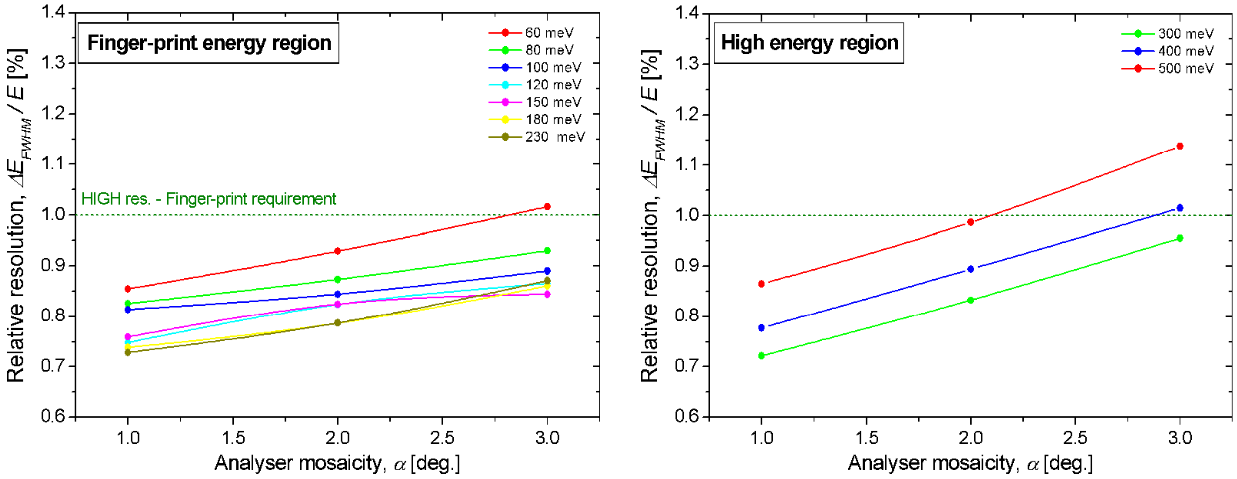


Fig. 1. Relative energy resolution ($\Delta E/E$) as a function of the analyzer mosaicity (α) at different energy transfers (E) in the VESPA Hi-Res. configuration (see color legend in the plots). The quantityΔE is calculated as the Full Width Half Maximum (FWHM) of the simulated spectral bands. Lines are only a guide for the eye.

So, also considering that not all the sources of energy resolution loss in the secondary flight path can be easily simulated via Monte Carlo methods, the team is very much inclined to select PANASONIC PGCX10 (with 1.5° nominal mosaicity) as the baseline to start looking for suitable providers. This choice will allow:

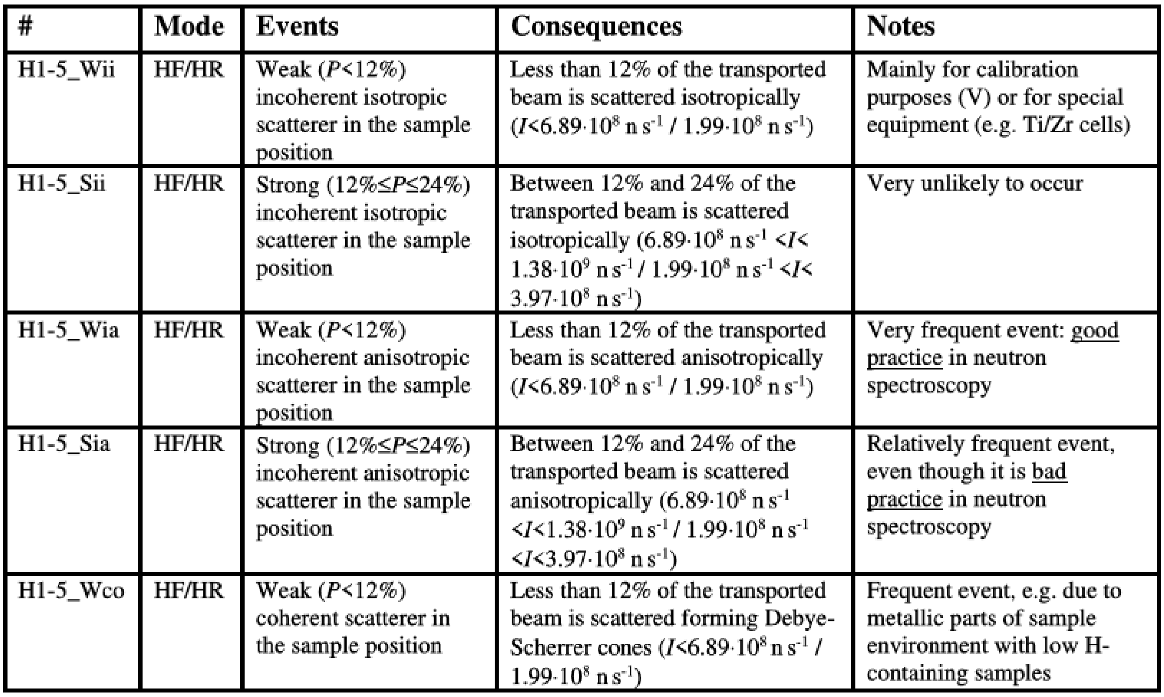
- to get a full resolution performance in both resolution modes (i.e. HR and High-Flux) starting from day-1, placing VESPA among the world-leading instruments in the “fingerprint” spectroscopic region,
- to contain costs,
- to leave space for possible unexpected resolution losses when installing the real components, as these losses are currently unpredictable,
- to avoid risks concerning the installation of components which are not yet fully developed.

In addition, it is worth noting that similar levels of analyzer mosaicity seem to be fully successful when employed on other crystal-analyzer indirect-geometry neutron spectrometers such as TOSCA at ISIS (α=0.8°) and VISION at SNS (α=2°).

As recommended in a previous STAP meeting (namely, that held on the 17th October 2019), VESPA team is also considering designing the mounting supports for the analyzer modules (also including Be filters and cold-head blocks) provided with manually adjustable features. This will allow to find the best alignment for the analyzer-filter-detector chain during the installation phase, enabling the optimal tuning of the neutron focusing which could impact on the finally achievable energy resolution.

2) Document *“H1 and H2 scenarios for the radiation shielding of VESPA”*

Although not yet submitted to ESS, the document *“H1 and H2 scenarios for the radiation shielding of VESPA”* has been first drafted and then finalized between May and June 2020. As requested by ESS, the scope of this document is to define the scenarios that are expected to drive the VESPA shielding design, and to set in place a simulation strategy to ensure that this shielding design is sufficient. H1 events are those related to normal operations, while H2 events are those which can be expected to happen with a frequency higher than 1/100 years. Considering the use of the VESPA beamline components, it is possible to separate the H1 events related to the first four components: light shutter, pulse shaping choppers, heavy shutter, and jaws (namely, H1-1, H1-2, H1-3, and H1-4), from those connected to samples and sample environment (H1-5).The reason of this separation is straightforward: all the complexity of the H1 recognition on VESPA is related to samples and their sample environment, which, due to the particularly rich user program ranging from chemistry to material science, can exhibit several different scenarios (see Tab. II for examples), including four scattering types: “weak incoherent isotropic” (e.g. thin vanadium), “strong incoherent isotropic” (e.g. thick vanadium), “weak incoherent anisotropic” (e.g. small H-containing samples), “strong incoherent anisotropic” (e.g. big H-containing samples), and “weak coherent” (e.g. thin aluminum or steel). On the contrary, the other components allow only a few degrees of freedom so that the list of their H1 events looks rather simple resembling that of other ESS beamlines.



#	Mode	Events	Consequences	Notes
H1-5_Wii	HF/HR	Weak ($P<12\%$) incoherent isotropic scatterer in the sample position	Less than 12% of the transported beam is scattered isotropically ($I<6.89\cdot 10^{8}$ n s^{-1} / $1.99\cdot 10^{8}$ n s^{-1})	Mainly for calibration purposes (V) or for special equipment (e.g. Ti/Zr cells)
H1-5_Sii	HF/HR	Strong ($12\%\leq P\leq 24\%$) incoherent isotropic scatterer in the sample position	Between 12% and 24% of the transported beam is scattered isotropically ($6.89\cdot 10^{8}$ n s^{-1} $<I<$ $1.38\cdot 10^{9}$ n s^{-1} / $1.99\cdot 10^{8}$ n s^{-1} $<I<$ $3.97\cdot 10^{8}$ n s^{-1})	Very unlikely to occur
H1-5_Wia	HF/HR	Weak ($P<12\%$) incoherent anisotropic scatterer in the sample position	Less than 12% of the transported beam is scattered anisotropically ($I<6.89\cdot 10^{8}$ n s^{-1} / $1.99\cdot 10^{8}$ n s^{-1})	Very frequent event: good practice in neutron spectroscopy
H1-5_Sia	HF/HR	Strong ($12\%\leq P\leq 24\%$) incoherent anisotropic scatterer in the sample position	Between 12% and 24% of the transported beam is scattered anisotropically ($6.89\cdot 10^{8}$ n s^{-1} $<I<1.38\cdot 10^{9}$ n s^{-1} / $1.99\cdot 10^{8}$ n s^{-1} $<I<3.97\cdot 10^{8}$ n s^{-1})	Relatively frequent event, even though it is bad practice in neutron spectroscopy
H1-5_Wco	HF/HR	Weak ($P<12\%$) coherent scatterer in the sample position	Less than 12% of the transported beam is scattered forming Debye-Scherrer cones ($I<6.89\cdot 10^{8}$ n s^{-1} / $1.99\cdot 10^{8}$ n s^{-1})	Frequent event, e.g. due to metallic parts of sample environment with low H-containing samples

Tab. II: Example of VESPA H1 events related to samples and sample environment (i.e. H1-5). Symbols **Wii, Sii, Wia, Sia,** and **Wco** stand for the scattering type: “weak incoherent isotropic”, “strong incoherent isotropic”, “weak incoherent anisotropic”, “strong incoherent anisotropic”, and “weak coherent”, respectively.Symbols**HF** and **HR** define the High-Flux (also known as Low-Resolution) mode and the High-Resolution mode, respectively. The values of the intensities *I* at sample position reported are obtained from *McStas* simulations of the VESPA spectrometer in both operational modes.

As for H2 events, those related to the first instrument section (H2-A), i.e. from moderator to sample area (excluded), are by far the most numerous since several likely accidents can happen in the primary spectrometer with a frequency larger than (or equal to) 1/100 years. Nevertheless, some of them are rather trivial since their practical effect perfectly overlaps with that of a corresponding H1 event.

However, moving to the sample area, we made a list of H2-B events for VESPA obtained assuming four types of likely accidents, where the transported neutron beam is intersected by:

a) large lumps of metal (e.g. an aluminum or steel block about 4 cm thick), typically fallen off sample environment pieces of equipment.
b) An overabundant hydrogen-rich sample (conventionally represented a 1 cm-thick polyethylene block).
c) A mass of frozen nitrogen from air which has accidentally flooded the VESPA closed-cycle refrigerator. In the sample area it could reach a thickness of about 15 cm.
d) The typical γ-ray production accident happening in a neutron scattering facility, which consists in a standard sheet of cadmium for neutron application (i.e. 2 mm thick), misplaced in the middle of the sample position and, consequently, irradiated by the transported neutron beam.

On the contrary, as for the H2 events related to the last section of the instrument (i.e. H2-C), from sample area (excluded) to detectors, the scenario looks simpler since this part is fixed, sealed, and bolted, with no access during the standard spectrometer usage.

These proposed scenarios will have to be complemented with the calculations of the so-called “neutron dose maps”, obtained through dedicated Monte Carlo codes (e.g. MCNP), which will verify if the actual shielding model is able to guarantee the 1.5 μSv/h value (including a security factor 2) for all the H1/H2 events and, in case it is not, they will help to implement the required changes in the shielding design.

3) VESPA instrument design and procurement: the overall project status

VESPA instrument accessed “Phase 2” (i.e. detailed design and procurement) in June 2019, but only in July 2020 the related Technical Annex and the Agreement on the rest of the project were finalized by the three partners [namely, ESS, CNR (Italy), and INFN (Italy)]. While the VESPA project was still waiting for the definition and the agreement on the contractual aspects governing this partnership, in spring 2020 various issues caused by the COVID-19 pandemic lockdown suggested reconsidering some of the ESS timelines and milestones previously presented, especially for the in-bunker access. Based on what has been recently shown in the Neutron Scattering Systems Master Schedule ver. 4.3 during the latest IKON19 meeting (28th-30th September 2020), the begin of the Hot Commissioning and Early Science for VESPA is expected in Q1/2026, with the in-bunker access slot planned in Q1/2025. At the moment, the opportunity to join the newly proposed ESS common projects is being discussed at the CNR top management level and leads us to consider another update of the project plan timing and tasks prioritization.
The status of the design of the main subsystems is presented in the following paragraphs.

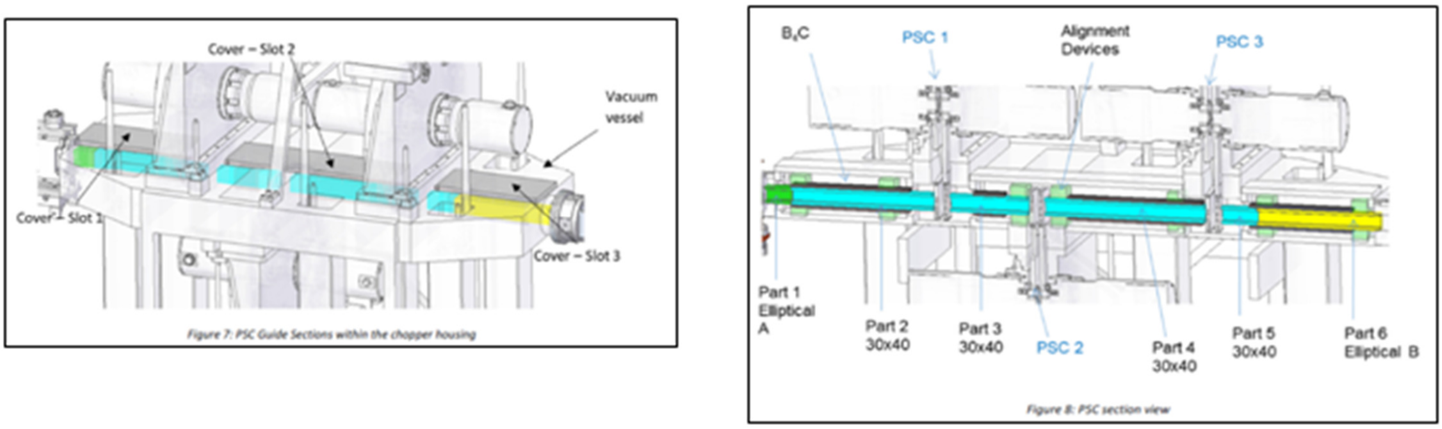
A) Instrument neutron guides

The design of the instrument neutron optics is now complete. After an accurate investigation and a performance improvement of the delivered neutron flux, the profile of the guide has been completely defined and the neutron guide has been engineered, producing a document with all the specification details useful for the related tender to be made for purchasing the VESPA guide on the market.
The preferred procurement strategy is to outsource the system as a turnkey contract including detailed design, manufacturing, and the installation at the ESS site of the entire subsystem:

- neutron optics,
- guide housing,
- alignment devices,

- remote handling features for in-bunker components,
- supporting structure,

Fig. 2. VESPA neutron guide details related to its pulse-shaping chopper part (left panel), and pulse-shaping chopper disks (right panel).



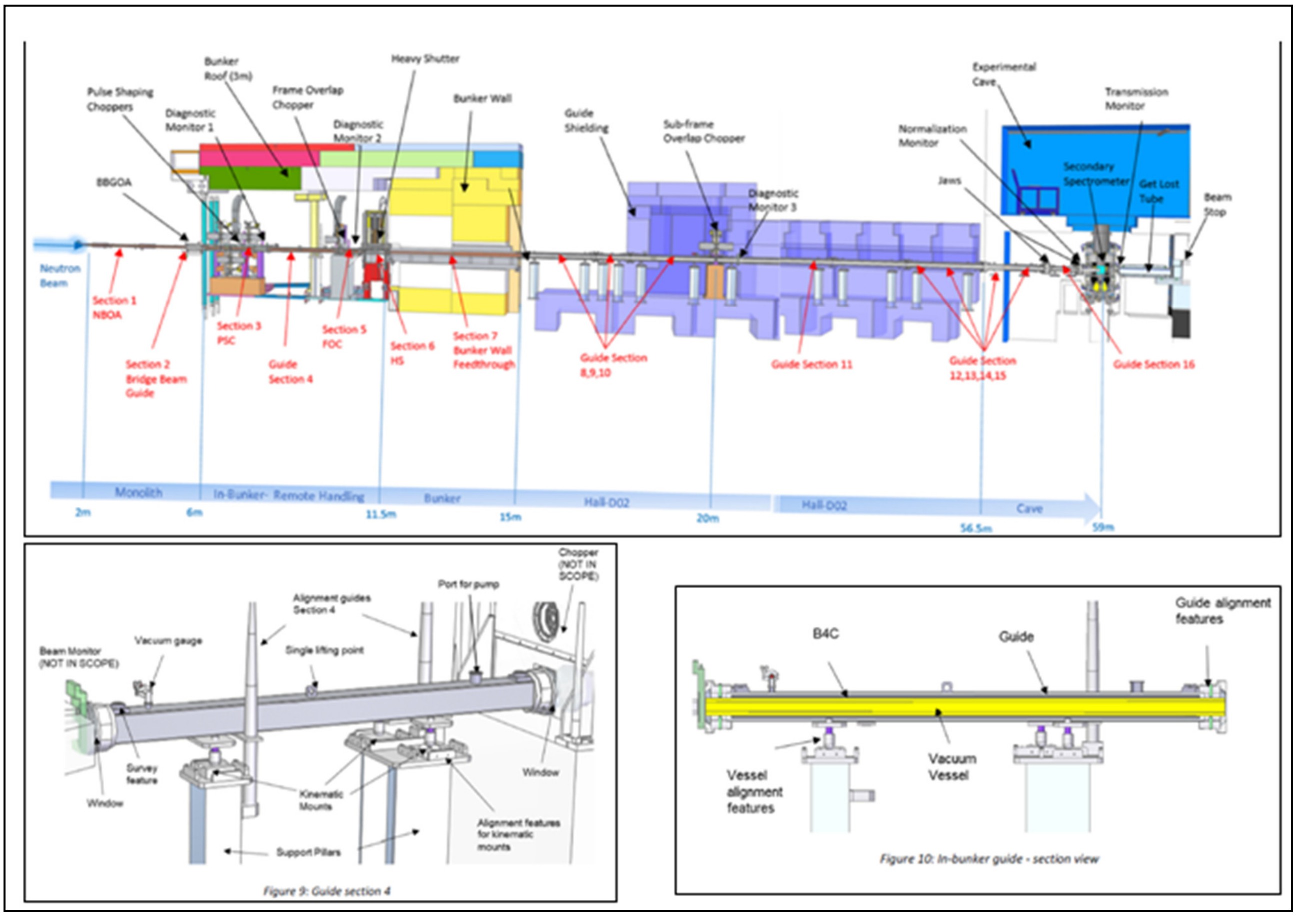


Fig. 3. The overall VESPA neutron guide system (upper panel), and its details related to the in-bunker part (lower panels, left and right).

Within the neutron guide subsystem, a preliminary design of the so-called “heavy shutter” has been also defined, verifying its capability to stop the transported neutron beam with a total component length of about 1.1 m. The neutron guide system and the heavy shutter will be part of the same procurement procedure as outsourced components, for which detailed design, manufacturing, and installation will be provided by external suppliers. A Call for Tender Verification (CTV) for this batch is expected to be held in June 2021.

Fig. 4. VESPA heavy shutter.

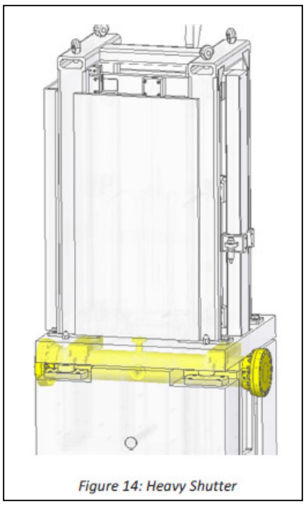


Figure 14: Heavy Shutter

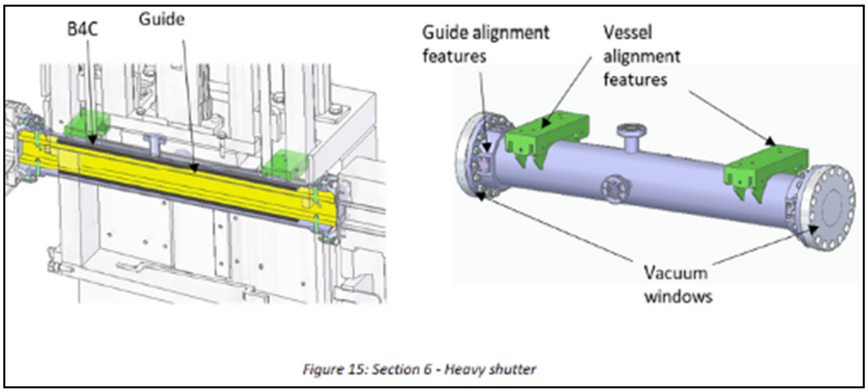


Figure 15: Section 6 - Heavy shutter

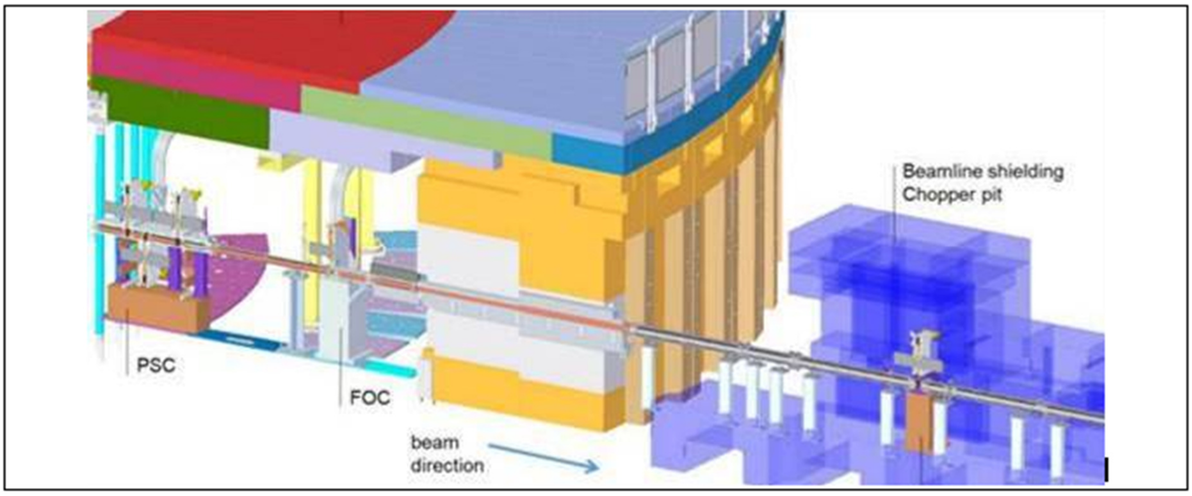
Fig. 5. Other details related to the VESPA heavy shutter.

B. Beamline shielding

VESPA instrument was part of the preliminary phase of the ESS common project related to the beamline shielding design. Dr. Jimmy Scionti, a new scientist of the VESPA instrument team, joined the ESS staff for a year to support and complete the neutronic model for the VESPA radiation distribution. A preliminary design and an economic offer were presented by ESS to CNR (Italy) and are now under discussion with the management, so the team is waiting for a feedback and some instructions on how to accomplish this task. Dr. Scionti is now developing a model of the radiation distribution along the instrument to define possible dose maps around the cave and the sample area and set up an adequate shielding. The beamline shielding will be provided as an external supply, and a CTV meeting is expected to be held in March 2021.

C. Chopper system

With the design of the neutron-beam delivery system, the instrument chopper suite has been defined and a preliminary engineering design has been presented. The detailed specifications will be submitted to the selected supplier as soon as the internal procurement process is defined. The considered procurement strategy is to outsource the detailed design, the manufacture, the delivery, and the installation at the ESS site of the VESPA chopper system.The availability of suppliers is unfortunately quite limited: AIRBUS S.A.S. is available for the supply of the entire suite even though its cost estimates considerably exceed the assigned budget. The ESS chopper team has also been considered for providing the present subsystem, but they expressed some concerns about their capability to produce disks exhibiting an 800 mm-diameter. In any case, this subsystem will be surely provided as an external supply, and a CTV meeting is expected to be held in April 2021.



(FOC) inside the bunker, plus the sub-Frame-Overlap Chopper in a dedicated chopper pit outside the bunker.

D. Analyzers, detectors, and sample environment

The analyzers of the VESPA instrument are based on a focusing design with several HOPG tiles arranged on a parabolic support. The analyzer design is now completed in terms of neutron physics; while a suitable engineering has been defined only for the individual components, also including some performance tests on materials that have been carried out in 2019. Namely, graphite tiles have been preliminary tested under neutron beam, while the glued assembly of these tiles on supports made of different materials has undergone a study of both its mechanical and neutronic performance. Similar tasks will be also accomplished on Be filters alone and, finally, on the full chain composed of HOPG tiles – Be filters– detector arrays. Preliminary contacts with the beryllium suppliers have confirmed the availability of the material with the desired grade and the possibility to cut it in slices of the required shape.

The final mechanical arrangement of the support structure and its integration with the vacuum vessel containing the sample and the VESPA-dedicated closed cycle refrigerator is pending, waiting for the experimental tests on HOPG, Be filters, detector arrays, as well as the final design of each component belonging to this subsystem. According to the project plan, the present subsystem will be developed in house, and an Interface Design Review (IDR) meeting is expected to be held in July 2022.

E. Experimental cave, control hutches, and services

The development of the experimental cave design is influenced by the analyzer one, as the spaces and the structures required by the secondary spectrometer (including sample vessel and detector arrangement) determine the design of the lower and upper cave. A general layout for the instrument backend is defined as follows, containing:

- a lower experimental cave where analyzers and detectors are installed,
- an upper cave with access to the top-loading sample vessel where either a sample stick or a sample changer can be inserted,
- an area dedicated to sample preparation,
- a control hutch with six working stations for users and instrument scientists.

Services and related routings are not yet defined in detail, and the electrical design for the instrument is only in a preliminary stage.The components of this subsystem will be procured from external suppliers: a CTV is expected in March 2021 if the missing inputs about the secondary spectrometer and the neutronic calculations for the cave shielding and beam-stop are made available in time.

The VESPA Team