30th September 2021

Spectroscopy STAP meeting

VESPA spectrometer: brief report on the activities done between early May 2021 and late September 2021

The present document is a brief report dealing with the activities of the VESPA team performed in the period between early May 2021 and late September 2021, i.e., essentially from the previous Spectroscopy STAP meeting (on 12th/04/2021) until now. We will focus on the three following points, including a reply to the issues contained in the latest report by the ESS Spectroscopy STAP panel (12th/4/2021):

1) Status of *Phase II*: detailed design and procurement for VESPA.
2) Advances in the secondary spectrometer and cave design.
3) Reply to the latest report of the ESS Spectroscopy STAP panel.

1) Status of *Phase II*: detailed design and procurement for VESPA

A brief, but still reasonably comprehensive, presentation of the Phase II status of the VESPA project aims to adequately respond to the following issues: **the present stage of the project**, **the timing for the next installation** (if any), **the current challenges**, and finally, **the possible delays**. In order to deal with this subject in an analytical way it is useful to represent the VESPA project status and timeline through some boxes, each of them related to an individual work package and containing information about the *Call for tender verification* (CTV) and the *Tollgate III* (TG3). The third work package, WP03, does not include a detailed box as it will be carried out in the framework of the ***Chopper system ESS common project*.**

WP01: Guide system

#	Description	Original date	Revised date
WP 01.3	Guides CTV	Jun-21	Jan-22
WP 01.4	Guide system + Heavy shutter specification ready	Jul-21	Feb-22
WP 01.5	Heavy shutter contract signed off	Mar-22	Nov-22
WP 01.6	Guide system supply contract signed off	Mar-22	Nov-22
WP 01.7	Guide system IDR (*)	Aug-22	Aug-22
WP 01.8	Guide system + Heavy shutter TG3 final	Oct-22	Oct-22
WP 01.9	Out-of-bunker guide system FAT (**)	Feb-24	Feb-24

(*) Intermediate design review; (**) Factory acceptance test.

WP02: Beamline shielding, cave, and hutches
(Part of the Beamline shielding ESS common project)

#	Description	Original date	Revised date
WP 02.2	Cave CTV	Mar-21	Dec-21
WP 02.3	Cave Specification ready (for INFN)	Mar-21	Jan-22
WP 02.4	Beamline shielding CTV	Mar-21	Mar-22
WP 02.5	Beamline shielding specification ready (for INFN)	Mar-21	Mar-22
WP 02.6	Cave supply contract signed off	Jan-22	Nov-22
WP 02.7	Beamline shielding supply contract signed off	Jan-22	Jan-23
WP 02.8	Cave IDR (*)	Mar-22	Jan-23
WP 02.9	Cave WP03/TG3.1	Jun-22	Feb-23
WP 02.12	Cave FAT (**)	Apr-23	Jul-23
WP 02.13	Cave IRR 1/TG4.1	Jun-23	Aug-23
WP 02.14	Cave delivered to ESS	Jul-23	Aug-23
WP 02.15	Cave installation start	Sep-23	Sep-23

WP03: part of Chopper system ESS common project

Communications between the VESPA team and the ESS Common Project team have been activated. An update concerning the time schedule for the detailed design is expected to be ready in the next weeks.

WP04: Analysers, detectors, sample environment equipment, motion control & automation

#	Description	Date
WP 04.1	Analysers, detectors, sample env., and motion control. Detailed design end.	Jul-22
WP 04.2	Analysers, detectors, sample env., and motion control IDR (*)	Aug-22
WP 04.3	Analysers, detectors, sample env. TG3.2	Oct-22
WP 04.4	Analysers, detectors, sample env., and motion control. Procurement & assembly in-house start: specification ready (for INFN).	Oct-22
WP 04.5	Analysers, detect. components: supply contract signed off	May-23
WP 04.6	All supplies delivered to ISIS Assembly Start	Sep-23
WP 04.7	Analysers, detectors, sample env., and motion control FAT (**)	Nov-23

In the last six months the VESPA team has been mainly engaged with various issues connected to the design of the primary part of the spectrometer, trying to prioritize the work on the related work packages as much as possible. In addition, some computational effort has been addressed to the optimization of the secondary part and of the shielding around the experimental station, a.k.a. cave shielding.

It is evident from WP01 and WP02 boxes that the project has suffered a substantial **delay** (roughly 10-14 months) due to the combined effect of a certain scarcity of manpower and, moreover, the complex interactions between the three Italian institutions involved in the ESS project: INFN (the Italian representative entity), ELETTRA, and CNR (which is actually managing the VESPA project). In particular, due to administrative reasons, all the procurement stages will start only in 2022, although the team has already finalized the technical specifications, has drafted the documentation for the guide system, and is going to complete the cave specifications in the next weeks. However, in the last six months the situation has improved in a noticeable way and so we are now able to outline the new time schedule for the completion of the TG3, as reported in the boxes above.
Finally, as far as challenges are concerned, we initially thought that the requirements for our wavelength frame multiplication choppers (WFM choppers: double disk, ∅=800 mm, freq.=154 Hz) might represent a technological challenge with respect to the standard WFM chopper performance. However, after a detailed discussion with the ESS experts it turned out that it was not exactly the case and that the ***Chopper system ESS common project*** could cope with all the VESPA choppers (i.e., 3 WFM choppers, 1 frame-overlap chopper, 2 sub-frame-overlap choppers).

2) Advances in the secondary spectrometer and cave design

Two main advances have to be noted and shortly presented: the **fine tuning of highly oriented pyrolytic graphite (HOPG) for the VESPA analysers**, and the **neutronic calculations for the biological shielding of cave and beamstop.**
As for the former issue we have carefully evaluated the impact of the HOPG mosaic spread (whether 1.5 or 2.3 deg. as from a preliminary selection) using *McStas* simulations for the so-called *High-resolution Configuration* of VESPA (see the left panel of Fig. 1). In addition, we have also verified the full access to the elastic line for both types of instrumental configurations (i.e., *High-resolution Configuration* and *Low-resolution Configuration*). This check is surely worth mentioning here since the accessibility of the elastic line was a question raised by the spectroscopy STAP panel last year. Some calculations are still ongoing in order to better evaluate the resolution of the elastic line as a function of the sample size, with the aim to explore the possibility for VESPA to have some modest QENS capabilities, which are, however, absolutely ancillary with respect to the inelastic ones.

Dealing with the neutronic calculations for the biological shielding of cave, we have performed some MCNP-X simulations on both the upper and lower parts of the VESPA cave. In Fig. 2 we have reported two dose maps of the **lower cave** assuming 600 mm-thick concrete walls.

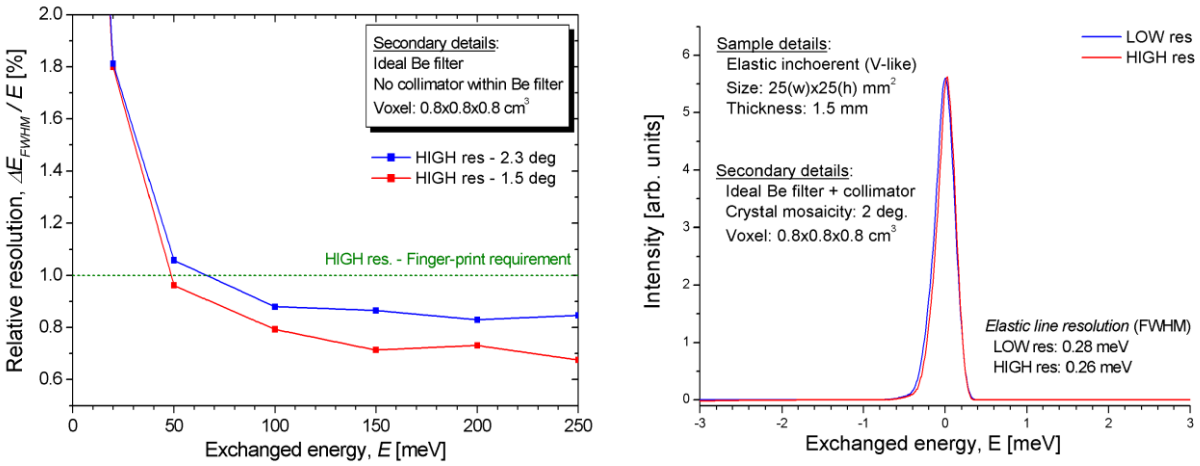

FIG. 1. (Left panel) simulated relative energy resolution (FWHM) as a function of the energy transfer for two selected values of the HOPG mosaic spread. (Right panel) Simulated vanadium-like spectrum for both instrument resolution settings.

One can visually verify in these maps that our design of the lower cave is fully compliant, as far as neutrons are concerned, with the 1.5 μSv/h dose limit.

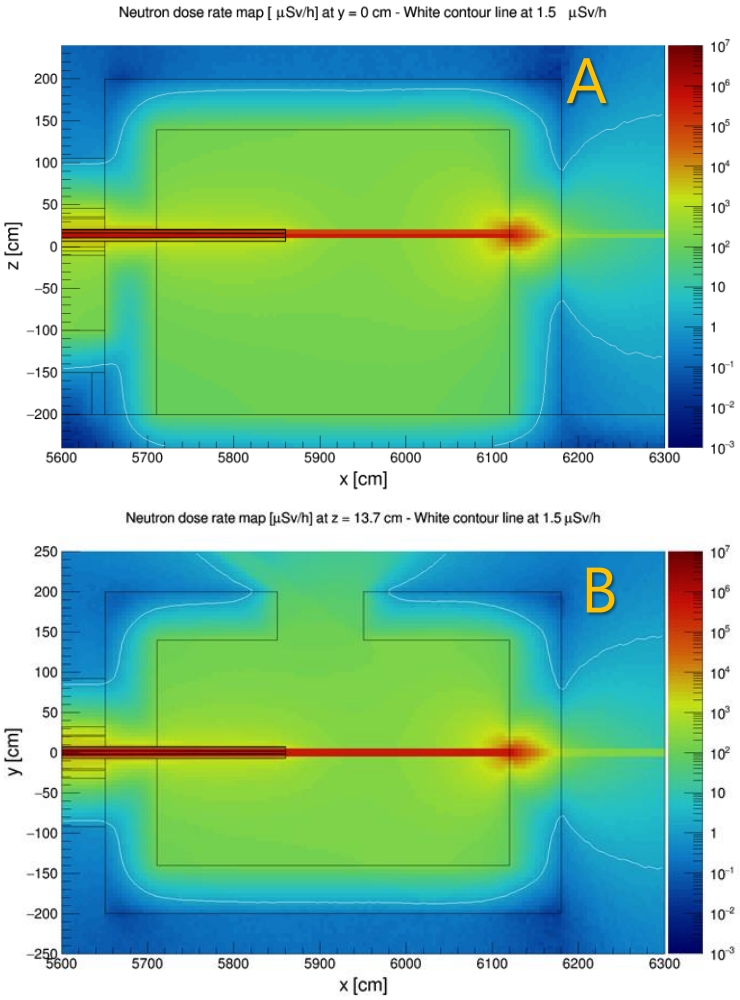

FIG. 2. Simulated neutron dose for the lower cave of VESPA: panel A represents the side view, while panel B the top view.

In the case of the **upper cave,** on the contrary, 300 mm-thick concrete walls seem sufficient to achieve the mentioned dose limit, both considering neutrons and gamma photons. Currently the team is also exploring the technical solutions for the design of the beamstop, which is not present in the dose maps reported in Fig. 2.

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

In the latest report (12th April 2021) by the ESS Spectroscopy STAP panel, the following four recommendations for the VESPA team were issued:

a. As long as VESPA does not have a T_0 chopper, the instrument will underperform when held to community expectations and facility ambition. The VESPA team could attempt to secure test beam time at TOSCA or VISION to make measurements of the full effect of a T_0 chopper. At VESPA, not having a T_0 chopper will also negatively affect the access to the elastic line. We recommend that the team estimate the effect of the full pulse of unshielded prompt gamma radiation from the flash pulse on a typical hydrogenous sample.

b. We are pleased to see that the choice of graphite analyser mosaic spread is being revisited. The simulation will be very beneficial in this case.

c. It is good to see that a redesigned cave will make more vertical space available for sample changers and instrument operations.

d. Since the team has spent some resources on the diffraction option for the instrument, we are wondering if the effect of hydrogen recoil has been considered in the simulation.

As for point "a.", related to the importance of a ***prompt pulse suppression chopper*** (also known as 'T_0 chopper') in the VESPA beam line, the team notices that this issue has already been dealt with in a number of ESS Spectroscopy STAP meetings. Unfortunately, it seems that the position of the STAP panel on one side, and that of the VESPA team on the other, had somehow crystallized and cannot be easily reconciled. For the sake of clarity, let us summarize our point of view on this important question:

i) We cannot exclude that the ESS Spectroscopy STAP panel is right, and a prompt pulse suppression chopper will be needed to produce high-quality scientific results on VESPA.
ii) For this reason, the beamline is already designed in such a way to make the installation of this device simple and straightforward.
iii) However, due to budget restrictions, we cannot afford to include a T_0 chopper from the very beginning of the VESPA user program (i.e., the so-called 'day one'). We will have to take the risk of a suboptimal spectrometer performance before the instrument upgrade.
iv) We fully appreciate the large and documented experience of some of the ESS Spectroscopy STAP panel members (e.g., as instrument scientists on vibrational spectrometers like TOSCA and VISION) and, for this reason, we have always pondered over their suggestions very seriously.
v) However, we have considered the fact that the TOSCA prompt pulse suppression chopper seems not to play a big role, at least according to the present TOSCA staff.

vi) Moreover, we have also taken into account the big differences between ISIS and SNS sources on one side, and ESS on the other, in terms of proton pulse, beam target, neutron pulse width, primary flight path length etc., concluding that at the present stage is practically impossible to provide an estimate of the effects of prompt gamma and fast neutron background on the vibrational spectra collection. It looks a tough job to simulate such effects, even with the most advanced codes like *MCNP, FLUKA* or *Geant4.*

Dealing with point “b.”, we can address the ESS Spectroscopy STAP panel to the new details about the VESPA analyser performance simulated via *McStas* and reported above in this document.

Moving to point “c.”, as mentioned in the previous sections of this document, we have to point out that the complete redesign of the cave, although started some months ago, has not yet been completed, since the VESPA team devoted most of its effort to the primary part of the spectrometer. However, we are sure that in the next weeks the VESPA cave will be fully redesigned.

Finally, dealing with point “d.”, we have to admit that our *McStas* simulations have so far been performed using only proton-free samples (i.e., $Na_2Ca_3Al_2F_{14}$ and CeO_2). However, the VESPA team is fully aware of the strong incoherent signal plaguing forward-scattering diffraction banks in the case of proton-rich samples. Dedicated diffraction simulations will be surely arranged for this kind of samples, even though our experience suggests that VESPA diffraction capabilities will be mainly focused on perdeuterated (or hydrogen-free) materials.

The VESPA Team