1st April 2021

Spectroscopy STAP meeting

VESPA spectrometer: brief report on the activities done between late October 2020 and early April 2021

The present document is a brief report dealing with the activities of the VESPA team performed in the period between late October 2020 and early April 2021, i.e., essentially from the previous Spectroscopy STAP meeting (Lund, 21st/10/2020) until now. Since the latest meeting, the VESPA team has recruited a new scientist, mainly devoted to shielding calculations and beam monitor design, and a new mechanical engineer. Owing to these new human resources, the team's work is currently focused not only on the design development of shielding, cave, and secondary spectrometer, but also on preparing the drawings and the documentation for the so-called *Call for Tender Verification* (CTV) for the first items to be procured: guide system, chopper system and cave/shielding. Moreover, a discussion at the level of the CNR top management about the participation in some of the ESS common projects, like those regarding choppers, shielding and electrical services, is still ongoing.

Leaving aside the detailed managerial and procurement/delivery aspects of the VESPA team's work (which could be hardly summarized here), 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 (3rd/11/2020):
1) Secondary spectrometer development: diffraction banks.
2) Update on the shielding design.
3) Reply to the latest report of the ESS Spectroscopy STAP panel.

1) VESPA secondary spectrometer development: diffraction banks

Although the diffraction capabilities of VESPA are considered "ancillary" with respect to its spectroscopic performances, they represent an important feature for the scientific success of the instrument, because users can simultaneously collect both types of data, i.e., a 0-500 meV energy transfer spectrum and a 0.4-3.2 Å *d*-spacing diffractogram in one shot, extracting structural and dynamical information even during kinetic experiments. The VESPA diffraction performance is expected to be quite interesting, even for the highly incoherent samples usually measured on this type of spectrometers. This is mainly due to the high resolution of the primary part of the instrument (up to 0.4% λ_0 in the so-called *HIGH res.* mode), the low ratio between secondary and primary flightpath ($L_1/L_0 \approx 1/52$), and the high neutron flux at the sample position (up to $8 \cdot 10^8$ n/s/cm^2 in the so-called *HIGH flux* mode) for a large bandwidth (0.4-4.7 Å), that is efficiently transported by the neutron guide from the ESS thermal moderator.

Based on what has been approved by the so-called *Tollgate 2*, VESPA will be equipped with one diffraction bank in equatorial position on "day-1" (see left panel of Figure 1), with the possibility to install other banks, either in the equatorial position or in backscattering, during the upgrade phase. In these last months, by means of *McStas* simulations, we performed a preliminary study to define the main features of the diffraction banks. At this stage of the project, our design efforts are aimed at maximizing the relative resolution and the accessible *d*-spacing range of the diffractometer without affecting the design of the spectrometer components. As a general overview of the performances of the VESPA diffractometer in the current configuration, in right panel of Figure 1 we report two diffractograms of an ideal $Na_2Ca_3Al_2F_{14}$ sample, commonly used as a standard for calibration purpose, simulated by the *McStas* code with no intrinsic line broadening (for details, see the caption of Figure 1 and Table I). The overall quality of the diffraction data seems quite satisfactory in terms of resolution, with a particular mention to the backscattering bank. It is necessary to highlight that the resolution of the diffraction patterns recorded by the equatorial banks can be further enhanced by increasing the incoming beam collimation using the double jaw sets placed in the final section of the guide. Indeed, with a reduced beam size of 10×10 mm^2, the *d*-spacing relative resolution can reach an almost constant value of 0.7% in all the *d*-range. With further design developments, it will be probably possible to add a collimator in the secondary flightpath to further enhance the resolution performance, as well as to find additional free space for increasing the detector surface of each bank, so to obtain a wider coverage of the *d*-spacing range. Moreover, we think that it could be interesting to explore the possibility to have an extra bank in forward scattering, to be installed in the upgrade phase of the instrument, in order to give access to the *d*-spacing region around, or even above, 4 Å. This is particularly useful in the complex chemical systems frequently analyzed by neutron vibrational spectrometers like VESPA.

Table I. Main features of a possible working configuration of the diffraction banks, assuming the *HIGH res.* setting for the primary spectrometer. For a rough estimate of the peak count rate in both instrument settings, we take as reference the most intense reflection of a $Na_2Ca_3Al_2F_{14}$ sample with a scattering power of about 10 % at 5 MW source power.

Bank (nominal angle) [deg.]	Sample-detector distance [m]	Detector surface [mm^2]	Scattering angle 2ϑ coverage [deg.]	Spatial resolution [mm]	Time resolution [µs]	Position sensitivity	Peak count rate (*HIGH flux* / *HIGH res*) [n/cm^2/s/%SP]	*d*-spacing range [Å]	$\frac{\Delta d_{FWHM}}{d}$ [%]
Equatorial (90)	0.8	280(w)×200(h)	80-100	8(w)×8(h)	10	Yes (optional)	$6\cdot10^3$ / $3\cdot10^3$	0.4-3.2	<2.0
Backscattering (161)	1.0	160(w)×160(h)	156-166	8(w)×8(h)	10	Yes (optional)	$4\cdot10^3$ / $3\cdot10^3$	0.4-2.4	<0.5

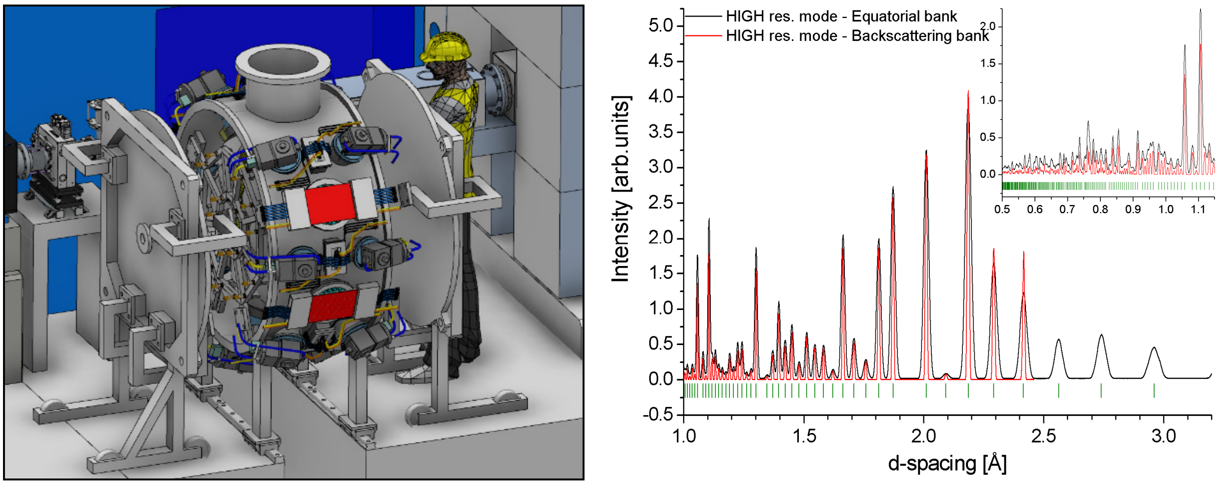

Figure 1. (Left panel) VESPA secondary spectrometer and vacum tank. The equatorial diffraction banks are highlighted in red. **(Right panel)** Simulated diffraction patterns in the *HIGH res.* mode of a $Na_2Ca_3Al_2F_{14}$ powder sample with a flat geometry [i.e. 25(w)×40(h)×4(t) mm^3] recorded by the equatorial bank (black line) and the backscattering bank (red line). The diffraction pattern, obtained by reducing the time-of-flight data coming from a 35×25 (equatorial bank) or 20×20 (backscattering bank) matrix, are arbitrarly renormalized to ease the comparison. Green bars mark the position of the Bragg reflections generated by the cubic crystalline structure of the $Na_2Ca_3Al_2F_{14}$ sample, characterized by a lattice parameter a=10.2531 Å. In this case we used a flat position sensitivy detectors [namely, 280(w)×200(h) mm^2 for the equatorial case and 160(w)×160(h) mm^2 for the backscattering case] characterized by a spatial resolution of 8×8 mm^2 and by a time resolution of 10 µs. The L_1 distance was set to 0.8 m and 1.0 m for the equatorial and backscattering bank, respectively.

2) Update on the cave shielding design

In the last months, a new *MCNP* model of the cave has been created. The first Monte Carlo simulations performed using this model showed that 60 cm thick concrete walls are sufficient to ensure the requested level of radiation outside the cave, set to a dose rate of 1.5 µSv/h. However, since these shielding calculations are requiring more computational resources than expected, the cave CTV has been officially postponed from March 2021 to the last quarter of 2021. In any case, we have verified that it is still possible to meet the milestone for the so-called *"first installation access"* to the instrument hall, expected for VESPA in September 2023. Moreover, ESS has recently announced that it is going to review its Master Schedule within the last quarter of 2021. So, consequently, other re-adjustments of the ESS (and VESPA) milestones are still possible.

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

In the latest report (3rd November 2020) by the ESS Spectroscopy STAP panel, the following recommendations (both general 1., and specific 2.-6.) for the VESPA team were issued:

1. Do the technical solutions match the instrument's scientific requirements? This is largely the case with a few exceptions such as the lack of a T_0 chopper at VESPA which is extremely damaging to the scientific program of the instrument. (…). Most instruments are severely compromised in what is defined as "day-1 scope" for *them. This includes strongly limited detector coverage (equivalently, analyzer crystals for VESPA), sample environment equipment (high-field magnet for CSPEC), lack of* T_0 *chopper (VESPA), and other details.*

2. It appears that some high-level managerial decisions (or lack thereof) are slowing down the project and we hope that these can be resolved between ESS and their partners.

3. The team has obtained budgetary quotes for the guide and chopper systems.

4. The team has conducted a study of the optimal choice for the mosaic of the graphite analyzer crystals. The STAP is concerned that the team's overall conclusion, to go for 1.5 degrees, is perhaps too fine.

5. It is good to see the progress on the secondary spectrometer. As for day-1, VESPA will start with 2 analyzer modules (from a total of 14), and the STAP advises to be careful and strategic with the placement of the first analyzer banks (forward vs. backwarddirection). It will be essential to have full access to the elastic line. The STAP also recommends a minimum path length for all neutrons through the Be*-filter of at least 10 cm (the drawing shared during the presentation indicated that it is around 9 cm in the current design).*

6. The cave roof appears to be too low in the present design. The team should re-think the space requirements in this area for sample changers and other equipment.

As for point "1.", which underlines the potential damage for the "day-1" scientific program of VESPA caused by both the lack of a T_0 chopper (a.k.a. prompt pulse suppression chopper) and a reduced angular detector coverage (0.75 steradian), the VESPA team can surely accept, at least partially, the concerns expressed by the STAP panel, even though, as we have remarked in our previous replies, the "day-1" configuration was discussed in detail between the ESS and CNR management and then approved by the so-called *Scope Setting Meeting* (Lund, 27th/10/2016), also in view of the severe budget constraints of the project. As a matter of fact, the planned instrument upgrade will include an increase of the angular coverage by a factor 7 and, if needed, will provide the spectrometer with a T_0 chopper in a dedicated pit which will be already prepared in the beamline for the "day-1". In this respect, it is important to note that the effect of the former part of the upgrade will be a substantial reduction of the collection time, but no additional instrumental capability will be added to VESPA. On the other hand, dealing with the latter part of the upgrade, i.e., the prompt pulse suppression chopper, it is exceedingly difficult for us to foresee if its presence is crucial, or simply useful, to cope with the spurious background issue. This uncertainty is due to the fact that the ESS neutron source is quite dissimilar from both the ISIS and the SNS ones in terms of pulse width, moderators and distances. So, in our case is not simple at all to take inspiration from other neutron vibrational spectrometers like TOSCA and VISION.

Point "2." contains topics which are related to the managerial layer of the VESPA project which we do not belong to. For this reason, we prefer not to comment on this point.

Point "3.": no reply is needed here.

Point "4." raises the important issue of the optimal choice of the HOPG mosaic spread and expresses the Spectroscopy STAP opinion that a mosaic value of 1.5 degrees is probably too fine, which means that the final neutron energy selection would be too strict causing an unmotivated reduction of the detected neutron flux. The VESPA team has taken the Spectroscopy STAP suggestion on this subject very seriously and is currently analyzing X-ray and neutron scattering measurements on Panasonic PGCX20 (1 mm and 2 mm thick), where it has been able to detect an effective mosaic spread ranging from 2.2 deg. to 2.6 deg. At the same time the team is performing new *McStas* simulations of the VESPA secondary spectrometer making use of this mosaic spread values in order to check the instrumental performance in terms of energy transfer resolution.

Point “5.”is related to two important issues concerning the secondary spectrometer (i.e., from sample to detectors). The former is about the access to the so-called “elastic line” ($\hbar\omega$=0) in the “day-1” configuration of the spectrometer with only 2 modules (out of the 14 modules planned for the final configuration). We can reassure the Spectroscopy STAP panel that special care will be devoted to ensuring the possibility to measure the elastic part of the spectrum, no matter if backscattering, forward-scattering or both positions are selected as the angular positions of the first 2 modules. As far as the Be thickness crossed by the scattered neutrons selected by the HOPG monochromators is concerned, we will use not a filtering slab, due to the presence of curved analysers, but, following the example of VISION, a sort of filtering wedge. This shape can be approximately characterized by four parameters: *inlet, outlet, thickness,* and *angle.* So far, our best simulations have provided the following figures for a reasonable compromise between performance, cost, and encumbrance: 1.5 cm, 5.1 cm, 14.7 cm and 17.10 deg. This choice corresponds to a *rejection rate* (defined as the average transmission over the 0.1-5.0 meV range divided by the average transmission over the >5.0 meV-range) of about $4.76\cdot10^3$, when the filter is placed at 2.5 cm from the graphite analyser. This rate is roughly equivalent to a 12 cm-thick slab in the case of a flat geometry, in perfect agreement with the Spectroscopy STAP panel recommendations.

Point “6.” deals with the design of the VESPA cave pointing out the insufficient height of the ceiling: a completely updated design of the instrumental cave has been produced in the last months. This has been mainly driven by the new shielding calculations of the cave walls and roofs. Within this work, special care has been devoted to optimizing the cave size and layout, also with respect to the experimental and technical needs, like clear space for the utilities (gas cylinders, handling system, etc.) and for the internal crane devoted to sample environment handling (e.g. sample changer).

The VESPA Team