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CSPEC DETECTOR RESCOPING

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1. INTRODUCTION

CSPEC is the cold chopper spectrometer of the European Spallation Source (ESS). CSPEC will serve diverse scientific communities, such as life science, magnetism, soft matter, energy and functional materials. CSPEC is optimised to harness the significant peak and average flux of the ESS while taking advantage of the low noise levels [1]. CSPEC is designed to enable *in-situ* and *operando* experiments, kinetic measurements (with a time resolution of minutes for transient phenomena or ms for stroboscopic time-resolved measurements), and to probe materials for which the synthesis route results in samples that are too small for current capabilities. A few examples include:

- Collective and quasiparticle excitations in frustrated compounds.
- Low lying excitations in quantum matter.
- Magnon -phonon hybrid excitations in multiferroic materials.
- Time dependence of the rotational and translational diffusive processes in enzyme catalysis.
- Dynamics of hydration processes and the structural relaxation of the glassy water.
- Time dependent phenomena of hydrogen storage in clathrates.
- Proton diffusion in metal organic frameworks.
- Operando studies of proteins such as those involved in photosynthesis.

To this aim, CSPEC necessarily relies on a high-performance detector.

1.1. Requirements

The CSPEC high level instrument requirements are reported in [1][2][3] and are the following:

- CSPEC will extract a cold neutron flux with an incident wavelength range $2 \leq \lambda \leq 20$ Å.
- The CSPEC guide shall extract flux with ± 1° divergence at 3 Å and more, for higher wavelengths.
- CSPEC shall be capable of energy resolutions down to and better than $\Delta E/E$ = 1.5% for wavelengths greater than 4 Å.
- CSPEC shall be capable of momentum transfer resolution $\Delta Q/Q$ = 2%.
- CSPEC shall provide a signal to noise of 10^5 at 5 Å. Signal to noise is defined as the peak of the intensity at the elastic line versus background obtained far away at a time of flight when the background level has been reached. These signal to noise values are valid with a 10% incoherent scatterer (*e.g.,* a vanadium sample) with dimensions of 4x2 cm^2 (height x width). Neutron spectroscopy is highly background sensitive, especially when the interest is on scattering functions which are weak and broad in both energy and reciprocal space (*e.g.,* to allow investigating the signatures of spinon pairs, spin-liquids, or the exact details of diffusional processes). The signal to noise level requirement is based on current state-of-the-art cold chopper spectrometers.
- For each impinging pulse on the sample with energy E_i, an energy transfer $\hbar\omega = 0.2\,E_i \leq E_i \leq \infty$ will be measured
- The full detector coverage will eventually cover $-30° \leq 2\theta \leq 140°$ and a vertical detectable range of ± 26.5° (3.5 m).
- Repetition Rate Multiplication (RRM) will be employed for all data sets with the cumulative use of adjacent incident pulses for incident energy wavelengths ≥ 6 Å, with small variations in energy and momentum transfer, to increase flux.

2. DAY 1 LIMITATIONS AND PROPOSED UPGRADE

Current day 1 plan for CSPEC detector comprises the production of 12 ILL-MultiTube (MT) modules (and 1 additional spare) of 32 tube each. However, only 7 modules will be filled with 2.5 bar of ^{3}He gas, providing an angular coverage of *ca* 5° ≤ 2θ ≤ 110° (Figure 1, purple sector), with full vertical detectable range (± 26.5°, 3.5 m).

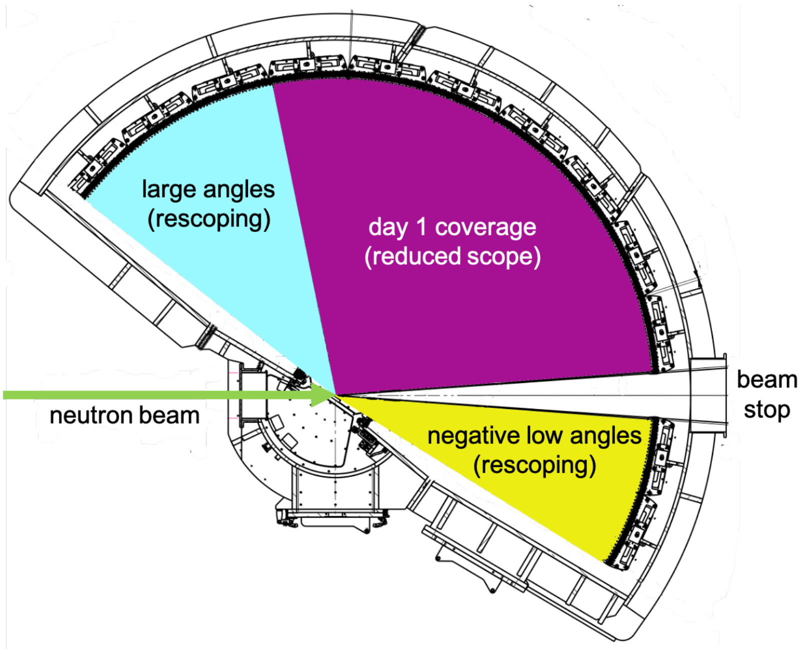

Figure 1 CSPEC detector tank view. The day 1 detector coverage (7 MT modules) is shown as coloured in purple and it equates to 58% of the full scope detector coverage of the instrument. The cyan and yellow sectors correspond to the MT modules at large angles and negative low angles, respectively. Such modules will be manufactured, but not filled with the detection gas.

2.1. Neutron detection efficiency

The pressure of the gas planned for day 1, 2.5 bar, will fulfil the requirement of an efficiency of at least 60% at *λ* = 4 Å, as agreed upon during the signing of the MultiGrid detector contract in 2016 [4]. However, when comparing the efficiencies provided by the 2.5 bar of the CSPEC day 1 detector with those of other world-leading instruments in its class (Figure 2), it is evident that CSPEC is underperforming, especially at shorter wavelengths. At the highest wavelengths, λ ≥ 10 Å, the differences are small, below 5%, and close to 1% above 15 Å. However, at λ = 2 Å, LET@ISIS and AMATERAS@J-PARC can detect neutrons almost twice as efficiently than CSPEC, while IN5@ILL and CNCS@SNS have efficiencies higher by factors of 1.5 and 1.6, respectively. CSPEC is designed to use a broad energy spectrum in the cold regime, and the region below 6 Å (highlighted in Figure 2) is still extremely important for all those studies that can use a relatively relaxed resolution, trading it for a wide kinematic range, unattainable at other types of neutron spectroscopy instruments. Setups using such incident wavelengths are in high demand during proposal rounds, and in this range the efficiency of CSPEC is *ca* 10-40% lower than that of the other instruments.

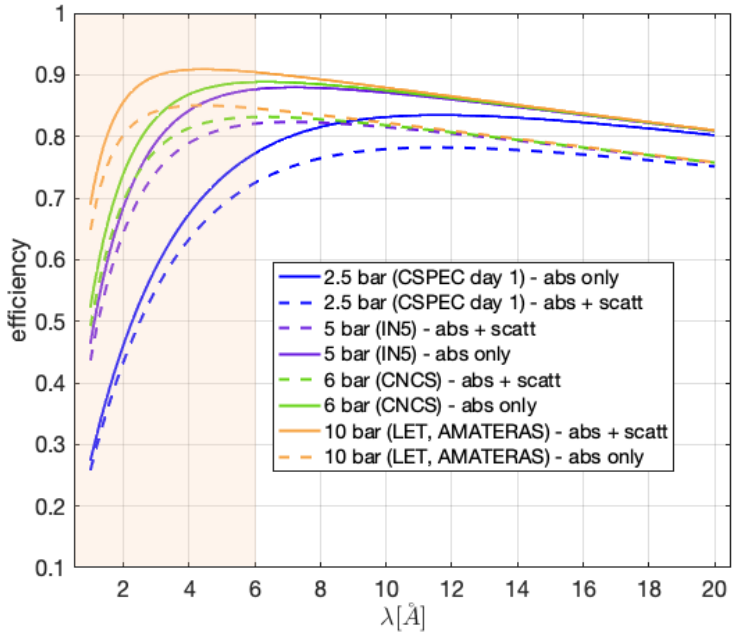

Figure 2 Efficiency of stainless-steel tubes filled with different ^3He gas pressures as a function of neutron wavelength. The expected efficiency for each pressure value should lie between the corresponding solid (both absorption and scattering events considered) and dashed lines (only absorption considered). At $\lambda \geq 10$ Å, the differences are small (below 5%), but at $\lambda = 2$ Å the efficiency of CSPEC is almost 2 times smaller than that of LET and AMATERAS, 1.6 times smaller than that of CNCS and 1.5 times smaller than that of CNCS. In the region highlighted in orange, below 6 Å, the efficiency of CSPEC is about 10-40% lower than that of the other instruments.

2.2. Kinematic range

The reduced angular coverage limits the available kinematic range, *i.e.* the area of the ΔE-Q plane that can be probed during a scattering experiment. Figure 3 shows the kinematic range for three selected incident wavelengths (2.5, 3.5 and 4.5 Å). The grey area comprised between the black lines represents the kinematic range for CSPEC day 1 angular coverage (purple sector in Figure 1). The green area is the gain in kinematic range obtained by enlarging the angular detector range to $5° \leq 2\theta \leq 140°$, corresponding to the sum of the purple and cyan sectors in Figure 1.

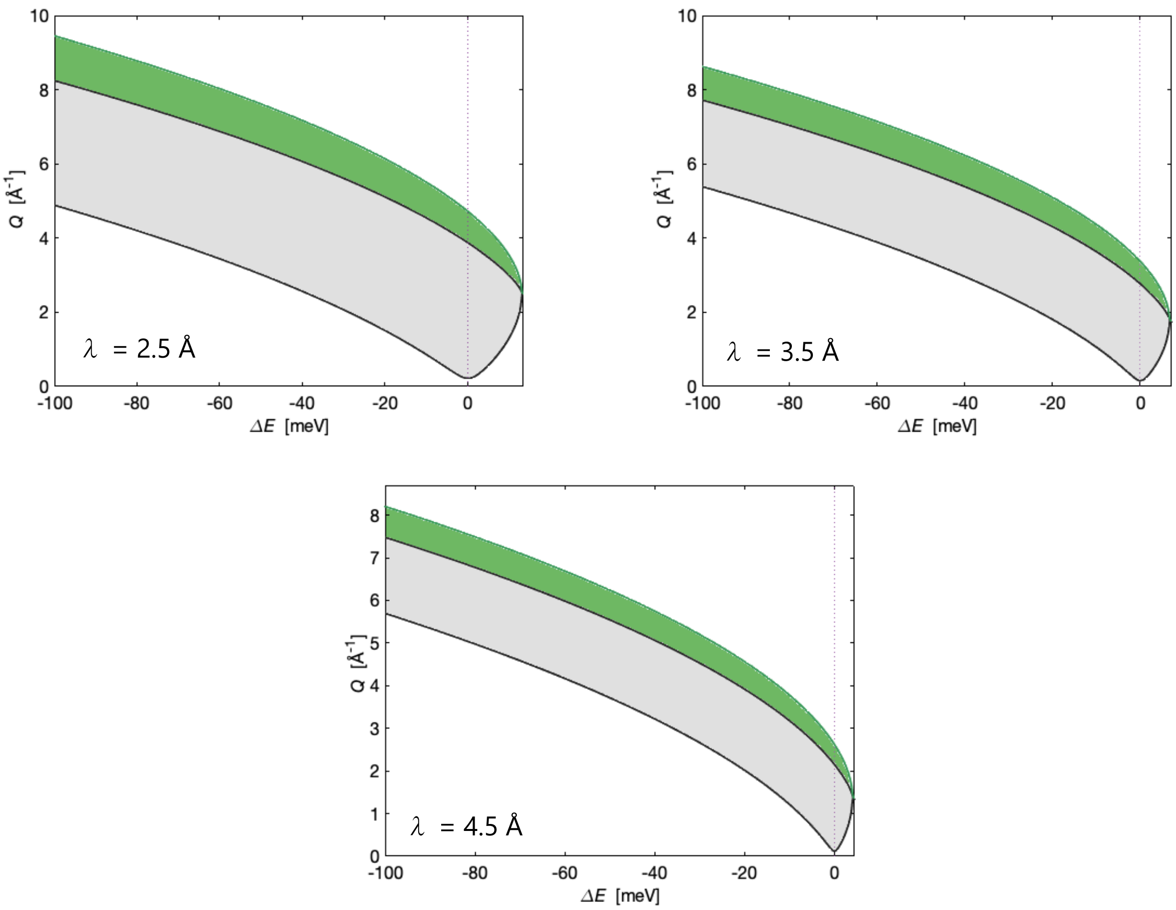

Figure 3 Kinematic range for incident wavelength equal to 2.5 Å (top-left), 3.5 Å (top-tight), and 4.5 Å (bottom). The grey area between the black lines represents the accessible area in the *ΔE-Q* plane accessible during the experiment for the day 1 angular coverage of CSPEC. The green area is the gain in kinematic range obtained by enlarging the angular detector range to full positive angular coverage.

An extended *Q*-range is fundamental to ensure a proper modelling and understanding of the dynamics in a variety of different systems, from soft mater to life science, to energy materials, to fundamental science, to magnetism. Figure 4 exemplifies the importance of an extended *Q*-range in different materials, from diverse scientific fields. The showed investigations, conducted on cold chopper spectrometers, pertain to H_2 hydrates [5], frustrated $Yb_3Ga_5O_{12}$ garnet [6], barium zirconate proton conductors [7], and ferrocene [8]. The maximum *Q*-value depends on the chosen incident wavelength according to the specific scientific case, and on the maximum angle covered by the detector. All the reported examples were obtained using incident wavelengths in the range 2 Å $\leq \lambda \leq$ 6 Å. In the reduced angular coverage of CSPEC day 1, many studies which are nowadays possible at operating would be feasible only with limitations that may prevent a comprehensive understanding of the investigated dynamics.

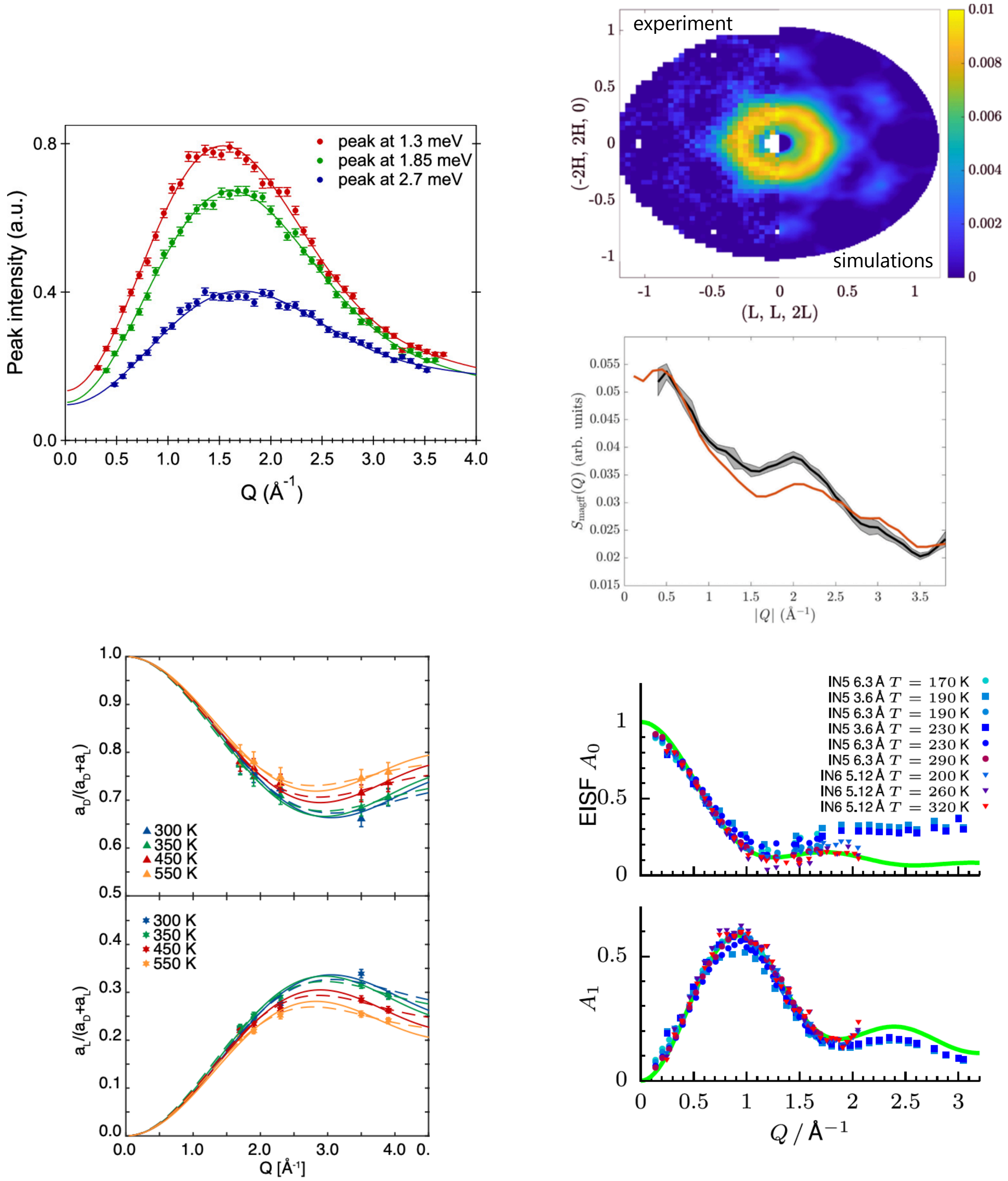

Figure 4 **Examples of investigations at cold chopper spectrometers in different materials. An extended *Q*-range, with max values depending on the selected incident wavelengths and on the maximum angle covered by the detector, is often needed in order to ensure a proper modelling of the parameters defining the dynamics. The investigated materials shown here are, from top to bottom and left to right: H_2 clathrates [5], frustrated $Yb_3Ga_5O_{12}$ garnet [6], barium zirconate proton conductors [7], and ferrocene. All the studies were done using incident wavelengths in the range 2 Å≤ λ≤ 6 Å.**

Moreover, we note here that the negative angular range (yellow sector in Figure 1) is needed in order to increase the quality of the signal at low *Q*-values, a region of outmost importance for *e.g.,* soft matter, magnetism, liquids and life science, and where the proximity of the direct beam makes the acquisition difficult.

2.3. First mitigation solutions: redistributing the ^{3}He gas in more modules

In order to mitigate this loss of capability, the CSPEC detector will have the possibility to adjust the gas pressure in the MT modules in the same way as at PANTHER@ILL. With such a technology, it will be possible to redistribute the ^{3}He gas in more MT modules, up to the full detector coverage. However, this will obviously drastically reduce the pressure in each module, and thus the efficiency of the detector, which is already suboptimal at lower wavelengths, *i.e.* the wavelengths needed for extended *Q*-range studies. Figure 5 shows the efficiency curves as a function of incident wavelengths for the ^{3}He pressure obtained by redistributing the day 1 gas from 7 MT modules to 10 MT modules (full positive angular range coverage, purple+cyan sectors in Figure 1) and 12 MT modules (full angular range coverage, purple+cyan+yellow sectors in Figure 1). As references, we report as well the efficiencies for 5 bar (pressure on IN5 and maximum gas pressure for which the CSPEC MT modules will be certified) and 2.5 bar (CSPEC day 1 gas in the reduced angular coverage of 7 modules). The loss of performance compared with 5 bar is stinking, especially at short wavelengths, with efficiency at 2 Å being about half (or even less for 1.46 bar).

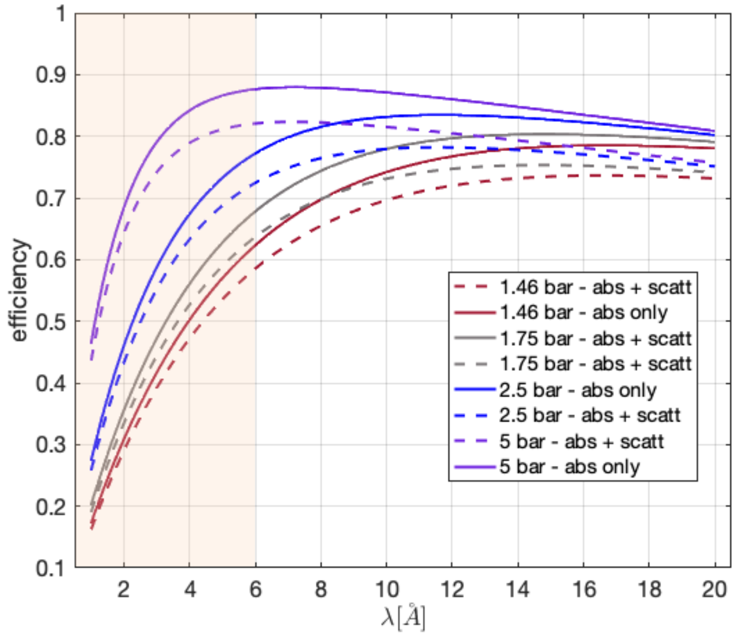

Figure 5 Efficiency of stainless-steel tubes filled with different ^{3}He gas pressures as a function of neutron wavelength. The expected efficiency for each pressure value should lie between the corresponding solid (both absorption and scattering events considered) and dashed lines (only absorption considered). The pressure of 1.46. bar is that obtained by redistributing CSPEC day 1 gas (2.5 bar in 7 MT modules) over 12 MT modules (full scope angular coverage, purple+cyan+yellow sectors in Figure 1); 1.75 bar is the pressure obtained by redistributing CSPEC day 1 gas over 10 MT modules (full positive angular detector coverage, purple+cyan sectors in Figure 1); 5 bar is the maximum pressure for the CSPEC MT modules, and the pressure used at IN5. In orange we highlight the "short wavelength" region.

2.4. Compared performance

In Figure 6, we compare the performance of some of the world leading cold chopper spectrometers at currently operating facilities with that expected on CSPEC with day 1 detector setup ($5° \leq 2\theta \leq 110°$ horizontal angular coverage, 2.5 bar of ^{3}He). The figure of merit (FoM) employed here is:

$$\text{FoM} = \text{Flux} * \text{Detector coverage} * \text{Efficiency}$$

The comparison is made for an incident neutron beam with incident wavelength λ = 5 Å and with ΔE/E = 3%. For CSPEC, we considered the single-pulse mode, without the use of Repetition Rate multiplication (RRM). By using RRM, CSPEC will gain significantly in flux. However, not all the scientific cases and setups will allow to use RRM to increase the flux, and it is also anticipated that RRM will take some time to become a standard operating mode. The ESS source power employed for this comparison is 2 MW. The flux values for CNCS@SNS, IN5@ILL and LET@ISIS were provided as private communications by instrument scientists at our partner's' facilities. More details are reported in [9], where a similar comparison is presented, but without including the detector efficiency in the employed FoM. From Figure 6, we can see that CSPEC with day 1 setup will have the same performance as IN5 and underperform with respect to CNCS. From the efficiency curves in Figure 2 and the discussion in the previous sections, we can infer that the loss of performance will be even more severe at some lower wavelengths. Also, we note that several months will be needed for the accelerator to reach the power of 2 MW.

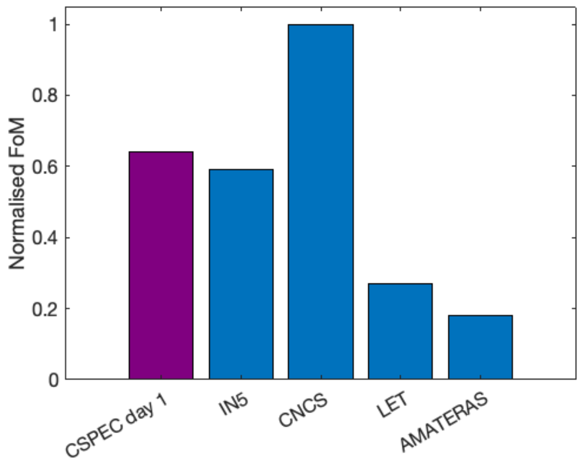

Figure 6 Comparison of the performance of CSPEC day 1 detector (2MW, single pulse) vs some of the current world leading cold chopper spectrometers.

In Figure 7, we expand the comparison by including the FoM for:

- CSPEC reaching full detector coverage by redistributing the day 1 gas into the 12 MT modules (labelled as *CSPEC full coverage, day 1 gas*), resulting in 1.46 bar in each MT module;
- CSPEC with full detector coverage and 2.5 bar of ^{3}He gas in each of the 12 MT modules (labelled as *CSPEC full coverage, 2.5 bar*);
- CSPEC with full detector coverage and 5 bar of ^{3}He gas in each of the 12 MT modules (labelled as *CSPEC full coverage, 5 bar*).

The FoM for such scenarios are calculated with the same conditions as for the CSPEC day 1 setup (*i.e.* single pulse, source power of 2 MW, λ = 5 Å with ΔE/E = 3%). For the sake of clarity, we include in this comparison only IN5 and CNCS, *i.e.* the two instruments with best performance according to the FoM employed here, as reference instruments. Although the full detector coverage 2.5 bar upgrade gives already a significant boost to the performance, it is clear that the optimal solution would be to upgrade to full detector coverage and 5 bar.

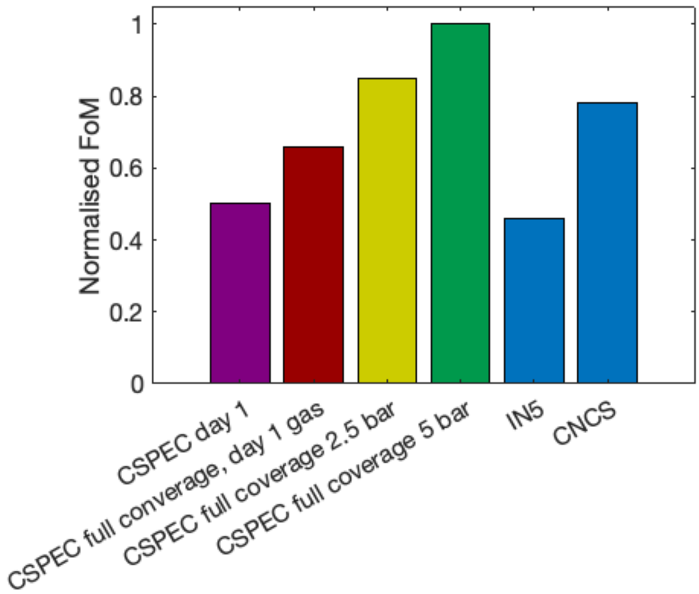

Figure 7 Comparison of the performance of CSPEC with different detector options vs some of the current world leading cold chopper spectrometers

3. COST ESTIMATES AND CONCLUSIONS

The CSPEC detector is currently planned to allow upgrades which can be implemented without disrupting the activity of the instrument and do not require additional personnel support. The costs of the presented upgrades are solely determined by the cost of the ^{3}He gas. The price of ^{3}He gas has fluctuated significantly over time, making it challenging to obtain a stable cost estimate or to secure "explorative" official quotes from suppliers. For the estimates presented in Table 1, the ^{3}He price is set at 2700 EUR/l, based on private communications with companies in May 2023.

Setup description	Estimated cost for the upgrade (2023 price) [kEUR]
Full coverage, 5 bar	6399
Full coverage, 2.5 bar	2025

Table 1 Cost estimates of the optimal upgrade, full coverage and 5 bar of gas, and a "minimum upgrade" of 2.5 bar in all the 12 MT modules.

The solution with 5 bar of gas in all the 12 MT modules is a straightforward upgrade which delivers the best detector performance achievable without modifying the detector or the detector tank. Therefore, this should be the target upgrade for CSPEC. However, if financial constraints impose limitations, it is possible to implement the upgrade in stages, ideally taking advantage of periods when the ^{3}He gas price is low.

As a final remark, the region below and above the beam stopper can be filled with smaller MT modules, or short single tubes, improving the low-Q region. However, this upgrade requires engineering work for its realisation and planning, and even in its exploratory phase. For this reason, it has not been prioritised at the moment and it is not part of this document. As a first rough approximation, 18 tubes (1-inch diameter) arranged in two sections of ca 1.25 m each (above and below the beam stop) can be considered. This corresponds to ca. 158 kEUR and 300 kEUR of ^{3}He for a pressure of 2.5 bar and 5 bar, respectively.

4. REFERENCES

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