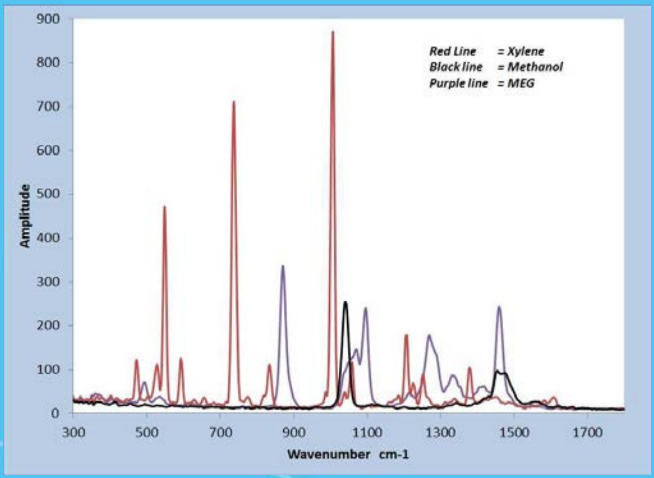
Signal to Noise Comparison of IS-Instruments Ltd High Throughput OEM Spectrometer and a Czerny Turner Instrument

July 2013



Presentation

www.is-instruments.com

EXECUTIVE SUMMARY

IS-Instrument's new range of High Étendue Spectrometers (HES) offers a greatly enhanced throughput or étendue over other commercially available spectrometer solutions. The instruments are compact with no moving parts. This increased throughput improves the flexibility of the HES OEM spectrometer, allowing them to be easily integrated into larger systems, particularly when studying diffuse sources. In turn, this makes the HES spectrometer a cost effective solution for a number of applications, including Transmission Raman measurements where light must be gathered from a 1 – 6 mm diameter sample.

When purchasing any OEM spectrometer or Raman spectrometer a number of factors must be assessed These include the type of measurements that are going to be made with the system, the resolution that is required for the observation, the flexibility of the instrument and the Signal to Noise measured when making a given observation. Additionally, engineering issues, maintenance and operational considerations and, of course, cost must also be taken into account.

In this technical note an initial investigation is made for the SNR that can be expected from IS-Instruments High Throughput Spectrometer (HES) compared to a Czerny Turner Instrument, taking account of both shot noise and detector noise effects.

The treatment shows that the SNR returned by the HES instrument, specifically when examining a diffuse source, can be up to 7 times greater than an equivalent Czerny Turner device studying the same diffuse sample. However, in certain conditions the more basic HES spectrometers can be more susceptible to detector noise than a Czerny Turner instrument, and so the treatment also includes an in depth look at the detector choices available in the HES range and how this maintains the HES advantage.

For more information contact IS-Instruments on

info@is-instruments.com

or visit our website

www.is-instruments.com

INTRODUCTION

When purchasing any spectrometer, a number of key criteria have to be considered. Typically these include the required spectral resolution, the spectral range, the type of measurement being made and the Signal to Noise Ratio (SNR) that can be achieved for a set of given measurement conditions. Secondary factors often include issues such as mass, ease of use and cost. The signal to noise comparison is often the most difficult to assess.

The HES ranges of spectrometers are designed to allow measurements of diffuse sources in a cost efficient package. This allows them to perform for example transmission Raman measurements in a compact package. In addition the high etendue of the instrument can also provide a superior SNR to be measured when using these devices.

In the specification of many spectrometers the SNR is often quoted by comparing the instrument noise floor and its digital dynamic range. This does not reflect real measurements where you must consider factors such the amount of light collected, the detector noise and the properties of the spectrum itself.

The amount of light collected is a function of three primary factors: The instrument's étendue or throughput, optical transmission and the detector Quantum Efficiency (QE). Often SNR treatments only consider the shot noise limited case (detector noise is negligible compared to the noise generated by the signal) and assume the effects of detector noise and, critically for diffuse sources, étendue are the same for all spectrometer designs. Other treatments consider all possible effects, including factors such as instrument drift, phase errors etc., which can make direct comparisons between systems difficult for a non-specialist in the field.

In this document the SNR is computed for IS-Instrument's HES spectrometer and a typical Czerny Turner system. The computation conducted takes account of signal strength and detector noise, but does not consider secondary instrument factors such as drift etc.

Generally, spectral measurement systems can be split into two categories: dispersive systems and interferometer based systems. Dispersive are simple, accurate and cost effective whereas interferometer based systems have a large étendue, allowing them to gather more light and are less susceptible to detector noise, but are more complex and can be very expensive.

IS-Instruments HES spectrometer combines many of the advantages of both of these types of systems. The instrument is simple, with no moving parts, and does not require expensive optical elements, while maintaining the étendue advantage offered by a Michelson interferometer.

COMPUTATION

The amount of signal gathered by a spectrometer from a diffuse source is given by:

$$S = \mathrm{QE}\ O_E A\Omega$$

Equation 1

where QE is the detector quantum efficiency, O_E is the instrument optical transmission and AΩ is the spectrometer receiving optical area solid angle product, also known as the instrument étendue. For a Czerny Turner system the AΩ product is given by the slit width and the instrument’s f/# number. This product is proportional to the spectral resolution of the instrument. For the HES spectrometer the AΩ product is given by the area of the dispersive element illuminated and the instrument’s field of view (FOV):

$$FOV_{HES} = \frac{2\pi}{R}$$

Equation 2

where R is the instrument’s resolving power. This is equivalent to the étendue of a Michelson interferometer and typically results in the HES having a 100 fold (or more) advantage in étendue over a standard Czerny Turner system of equivalent physical size and spectra resolution.

The QE of the instrument is clearly a function of the detector being used. For the purposes of this analysis it is assumed that both systems have the same detector. Clearly, when selecting any instrument the user must consider the detector very carefully in terms of both its sensitivity and noise. The optical transmission is a function of quality of the optical elements, the instrument design and the general manufacture of the product. For clarity, in this treatment it assumed that the assembly and the optical elements used in both designs are perfect. In order to achieve the étendue advantage the HES spectrometer sacrifices 50 % of the light in terms of optical transmission. Therefore the signal observed by the HES instrument (S_{HES}) compared to a Czerny Turner system (S_{CZ}), in identical observing conditions is:

$$S_{HES} \geq 50\, S_{CZ}$$

Equation 3

An imaging detector is used in both the Czerny Turner and the HES spectrometer so let us consider a signal spectrum with a line width significantly narrower than the instrument spectral resolution. The SNR for a standard dispersive system is therefore given by:

$$SNR_{CZ} = \frac{S_{CZ}}{\sqrt{S_{CZ} + N_D + N_R^2}}$$

Equation 4

where S_{CZ} is the signal strength in photons, N_D is the detector dark count and N_R is the detector read noise.

In the HES instrument the spectrum is recovered in Fourier space. The light returned from the signal source is recovered simultaneously for all spectral lines and is evenly distributed over all the pixels. Therefore the signal to noise is given by:

$$SNR_{HES} = \frac{S_{HES}}{\sqrt{S_{HES} + n(N_D + N_R^2)}}$$

Equation 5

where S_{HES} is the signal recovered by the HES spectrometer and n is the number of pixels over which the spectrum is distributed.

So in the case when studying a single spectral line the HES spectrometer is more susceptible to the detector noise effects. Therefore comparing the SNR returned by the HES spectrometer to a Czerny Turner system the following is true:

$$SNR_{HES} = \frac{50\ S}{\sqrt{50\ S + n(N_D + N_R^2)}} \tag{Equation 6}$$

So in the shot noise limited case ($S \gg N_D$; $S \gg N_R$) the HES spectrometer will enjoy a 7.07 improvement in the SNR over a Czerny turner instrument when performing identical measurements.

RESULTS

Single spectral Line – delta function

The first set of results takes the case when the target spectrum is a single spectral line that has width equivalent to the minimum resolution of the spectrometers, i.e. a delta function. In this case the Czerny Turner spectrometer will observe the entire signal in a single pixel on the spectrometer's detector. This represents the worse-case scenario for the HES when comparing with a Czerny Turner system.

There are three basic models of the HES spectrometer. The primary difference between each is the detector used. Simulations are conducted for low signal regimes of with 10 and 100 photons per second observed by the Czerny Turner instrument. As the photon levels increase above 10000 photons per second the instruments will become shot noise limited, at which the point the HES spectrometer will demonstrate a factor of 7 improvement in the SNR over a Czerny Turner system, as shown above.

These photon levels are chosen specifically so that the effects of detector noise can be more clearly observed for each of the spectrometers and, as such, are not practical but merely to demonstrate the comparison. In practice, a cooled CCD detector would need to be used for either spectrometer design.

The three types of detector adopted by the HES spectrometer are an uncooled, cost effective CMOS device similar to that found in a mobile phone. The second camera is a good quality, cooled CCD where the dark noise is signifcantly reduced, equavilent to the IVaC camera offered by Andor Scientific. The final system is a high quality, cooled CCD, equivalent to the Andor IDUS 420 system.

A summary of each configuration examined is presented within Table 1.

Table 1 Simulation cases

	Signal photons/s observed by Czerny Turner spectrometer	Detector noise (e/pix/sec)		Notes
		Dark Noise	Read Noise (RMS)	
Case 1	10	0.3	5	Cost effective, uncooled CMOS detector.
Case 2	100	0.3	5	
Case 3	10	0.01	5	Mid range, cooled camera (-50 to -60 °C)
Case 4	100	0.01	5	
Case 5	10	0.003	3	Top range, cooled camera (– 80 °C)
Case 6	100	0.003	3	

For these initial comparsions it is assumed that the HES spectrometer has 1000 pixels in the horizontal direction and 10 in the vertical (so n = 10000). In theory the number of pixels can be redcued to 1 in the vertical direction, reducing the effect of the dark noise. In practice this is diffuclt to achieve in a compact design as the high étendue of the spectrometer limits the ability to focus the light into a smaller number of pixels without a complex optical arrangement. A second reason is concerned with phase effects, which can, in principle, distort the resulting spectrum. It should be noted that many high quality Czerny Turner sytems also have some pixels in the vertical direction, but for the case of this comparions the spectrometer is have only 1 pixel in the vertical direction. The number in the horizontal direction is not important for the Czerny Turner system, only the number of pixels the spectral line covers.

Figure 1 shows the resulting SNR for both the Czerny Turner and the HES spectrometer as a function of integration length for Case 1 (left) and Case 2 (right).

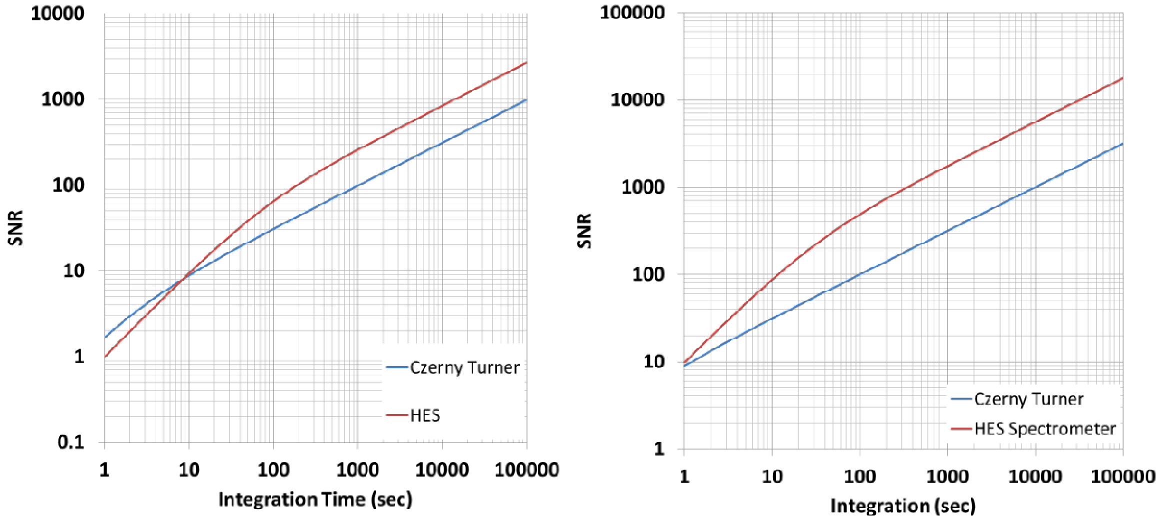


Figure 1 SNR comparison for an uncooled CCD: LH image = 10 photons observed per second; RH image = 100 photons observed per second. Red line = HES spectrometer performance; Blue line = Czerny Turner performance

In these scenarios the detector noise is very high, and thus has more of an effect on the HES system when the observed photon numbers are low. In Case 1 (uncooled CMOS, 10 ph/s), the HES spectrometer returns a higher SNR after 9s and then steadily outperforms the Czerny Turner system. In Case 2 (uncooled CMOS, 100 ph/s), the HES spectrometer outperforms the Czerny Turner over all the integration times simulated. After 10s the SNR returned by the HES is at least 2 times that of the Czerny Turner system, showing a considerable advantage even when detector noise is very high.

In both cases for low integration times, the noise that most affects the instrument's performance is the detector read noise. This is expected for CCD/CMOS based detectors.

Figure 2 shows the computed SNR for Case 3 (left) and Case 4 (right), where the detector dark noise is lower but the read noise is unchanged.

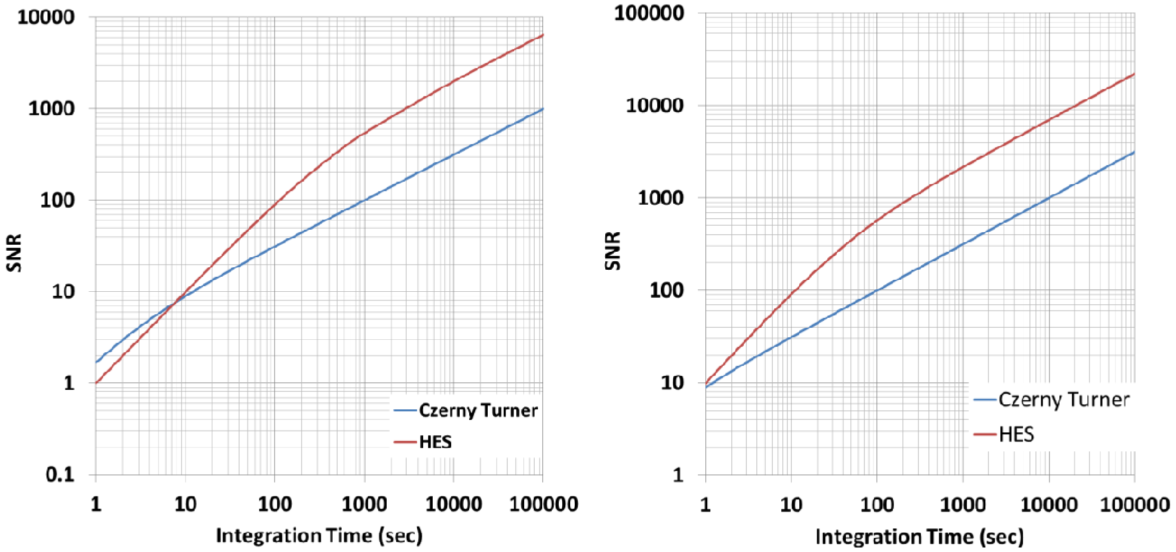


Figure 2 SNR comparison for a cooled CCD (case 3 & 4): LH image = 10 photons observed per second; RH image = 100 photons observed per second. Red line = HES spectrometer performance; Blue line = Czerny Turner performance

In Case 3 (cooled CCD, 10 ph/s) the Czerny Turner system has superior SNR for the first 7s but the HES then takes over as the superior device as the integration time lengthens. In Case 4 (cooled CCD, 100 ph/s) the HES spectrometer has a clear advantage across the complete range of simulations with the SNR returned by the HES up to 6 times greater than that observed in a Czerny Turner system.

Finally Figure 3 shows the expected performance of both spectrometers when a high grade, cooled CCD is used (Left: Case 5 and Right: Case 6).

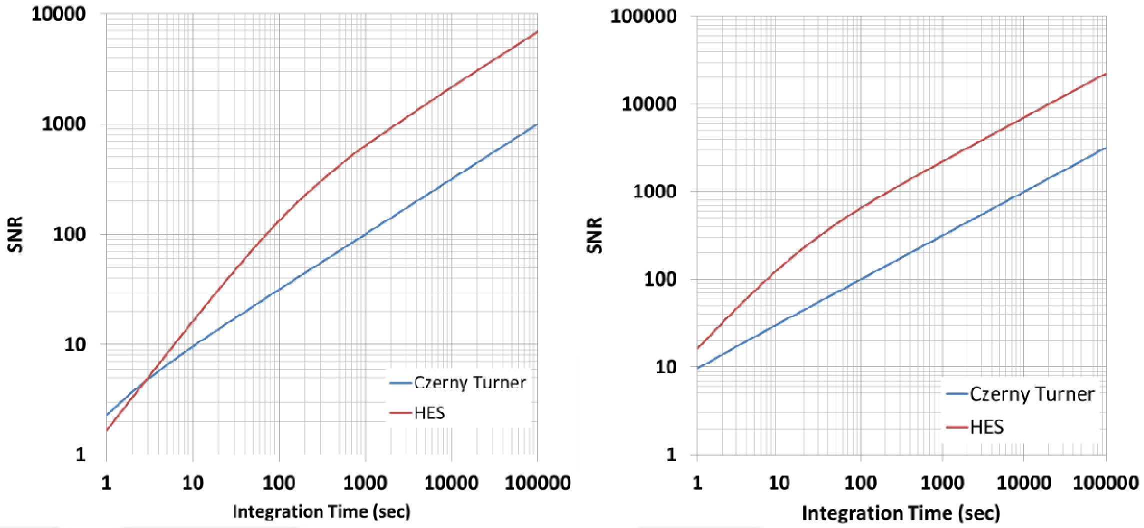


Figure 3 SNR comparison for a high quality cooled CCD (case 5 & 6): LH image = 10 photons observed per second; RH image = 100 photons observed per second. Red line = HES spectrometer performance; Blue line = Czerny Turner performance

In Case 5 (cooled, low noise CCD, 10 ph/s) the HES spectrometer provides superior SNR for measurements of 3s or longer. In Case 6 (cooled, low noise CCD, 100 ph/s) the HES provides a SNR of between 2 to 7.07 times that observed in the Czerny Turner for all the integrations times examined.

The Multiplex Advantage

Thus far the spectrum considered is a delta function and so the detector noise in the Czerny Turner system is at a minimum level. In reality, the spectrum recovered will have a larger finite width. In this case the HES spectrometer enjoys a partial multiplex advantage. As the spectrum spreads over more pixels, the noise from each pixel must be considered when using a Czerny Turner system, thus reducing the overall SNR that is observed. In the HES system all the light is distributed over the detector, therefore there is no equivalent effect. Thus it will return an improved performance over that generated by a standard dispersive spectrometer.

To demonstrate this effect consider the cases of a spectrum which is 10 pixels wide and 100 pixels wide. In order to compare the two systems more clearly the photon levels are set at 10 photons per second. It should be noted this is very low and, in practice, an uncooled detector would be poorly suited for this measurement. The resulting SNR when using the uncooled detector is given in Figure 4. This is an extreme case where the detector noise is very significant. However, the HES spectrometer maintains an advantage even for the smallest signals.

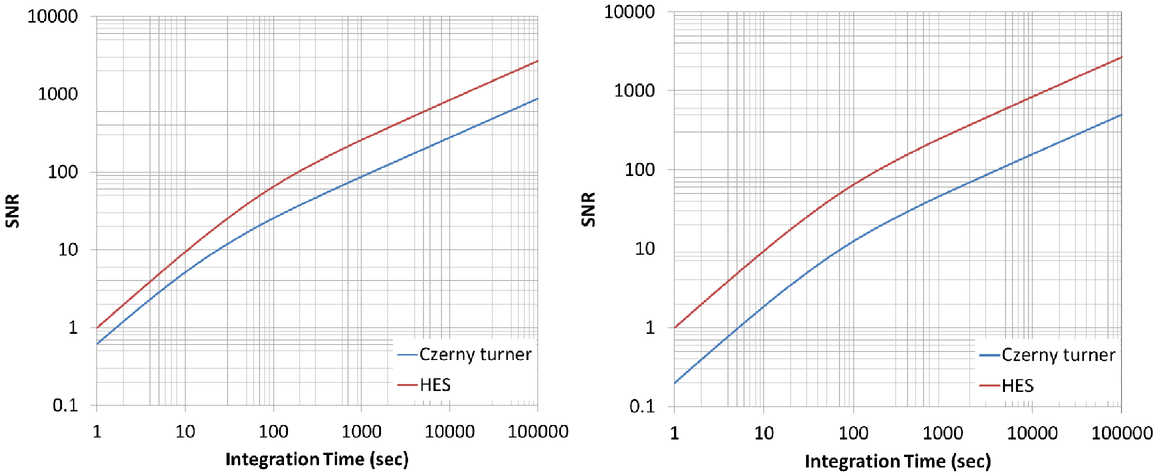


Figure 4 SNR comparison for an uncooled CCD with a count rate of 1 photon per second with different spectral widths: LH image = 10 pixel wide spectrum; RH image = 100 pixel wide spectrum. Red line = HES spectrometer performance; Blue line = Czerny Turner performance

For the 10 pixel case (LH image) the HES spectrometer enjoys a factor of 1.6 – 3 enhancement in SNR over the Czerny Turner system. However, given the very low signal level the detector noise is significant enough for the shot noise limited case not to occur. The RH image shows that once the spectral width increases to 100 pixels the throughput advantage offered by the HES system significantly improves the system performance. Even with this very low photon count (1 ph/s) the HES achieves a SNR over 5 times that observed by the Czerny Turner system, despite the detector noise dominating the performance.

In Figure 5 the simulations are shown using the cooled CCD with 10 (left) and 100 (right) pixel wide spectrums at the low count rate of 10 photons per second.

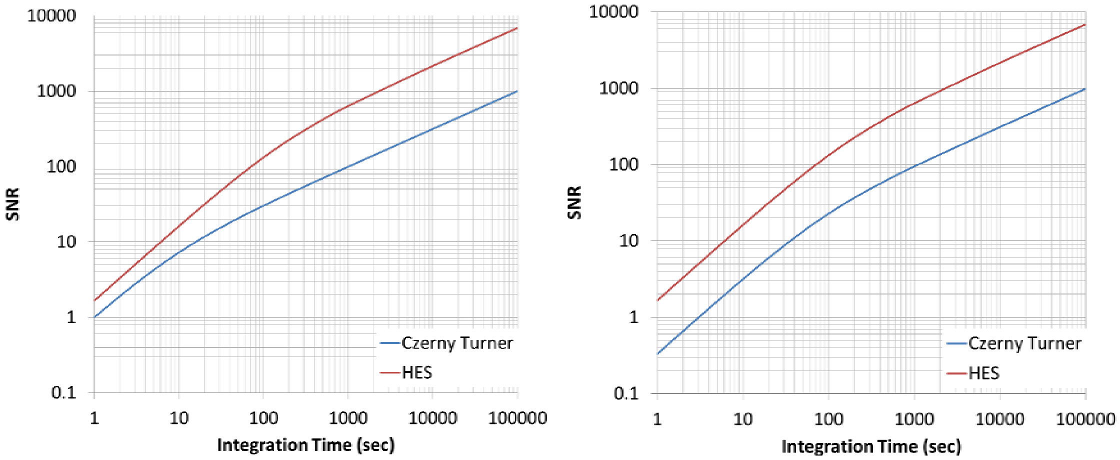


Figure 5 SNR comparison for a high quality cooled CCD with a count rate of 10 photons per second with different spectral widths: LH image = 10 pixel wide spectrum; RH image = 100 pixel wide spectrum. Red line = HES spectrometer performance; Blue line = Czerny Turner performance

The HES spectrometer provides a factor of at least 2 times improvement in SNR when the spectrum is 10 pixels wide for all integration lengths simulated. Unlike the uncooled CMOS simulated above the detector read noise never dominates at the long integration lengths and the shot noise limited case is achieved, giving the improvement of a factor of 7 in SNR.

For the case when the spectrum is 100 pixels wide and the low signal level (10 ph/s), the HES provides a significant advantage across the range from a factor of 5 to 7 improvement in SNR.

For completeness these simulations are repeated for a signal strength of 100 photons per second for both a 10 pixel and 100 pixel wide spectrum using the cooled and uncooled CCD.

The results are shown in Figure 6.

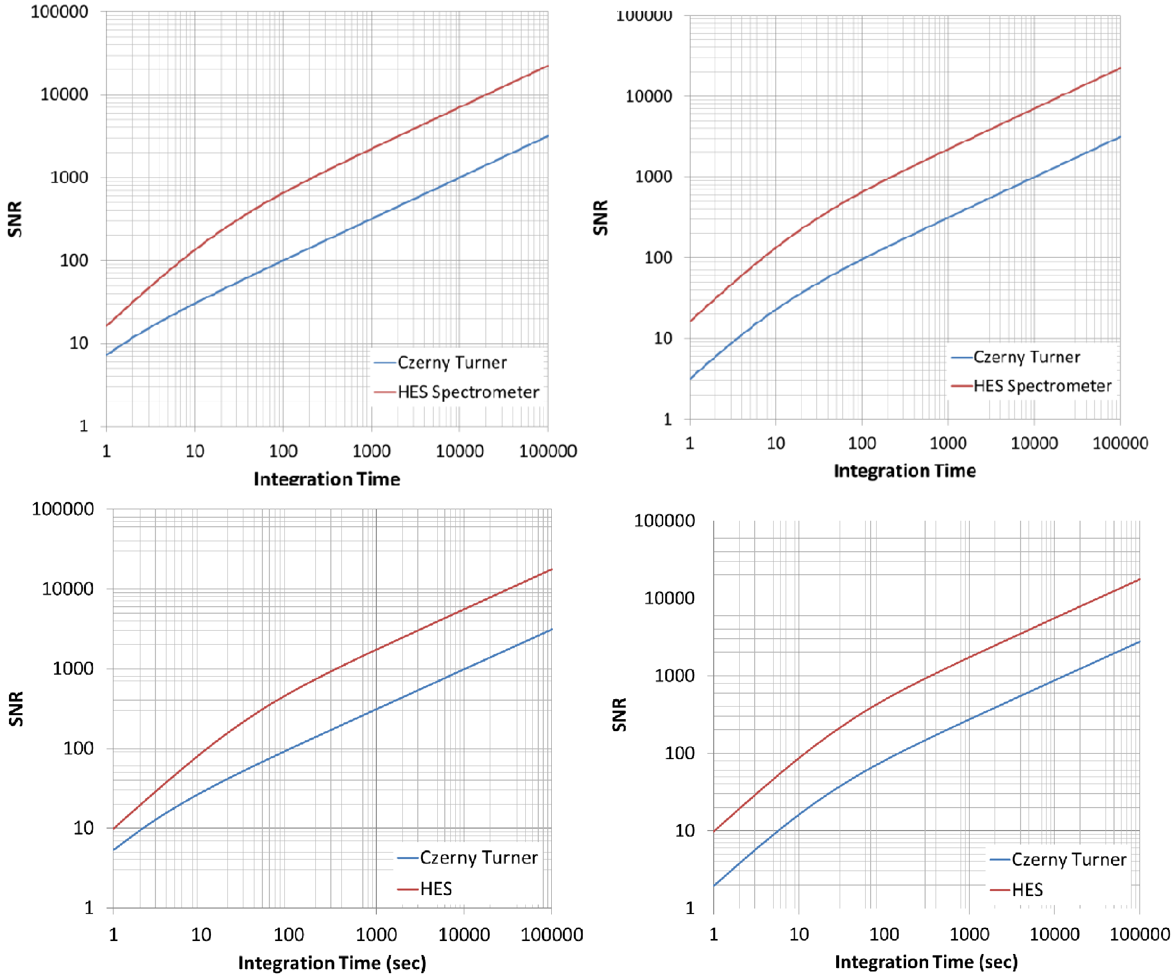


Figure 6 SNR comparison for a high quality cooled CCD (Top images) and uncooled CCD (bottom images) with a count rate of 100 photons per second with different spectral widths: TLH image = 10 pixel wide spectrum; TRH image = 100 pixel wide spectrum. Red line = HES spectrometer performance; Blue line = Czerny Turner performance:

All the results simulating the wider spectrum show that the HES shows a significant advantage, even when the detector noise dominates over the shot noise. This provides clear evidence that the system is well suited for applications with spectrums of variable width and complexity, such as Raman measurements. Another factor to consider, but not discussed in detail, is that all the noise from the spectrum is spread evenly over the acquired spectrum. This means that the noise in emission peaks (as in the Raman case) in proportionally lower, providing further improvements in the expected SNR. However, the opposite is true for absorption spectroscopy, where the noise for the valley will be increased by the same effect. In both cases these issues are small compared to the signal and detector noise.

Using Different Detectors

Thus far the performance of the different spectrometers has been considered assuming the detectors used in each option are identical. In practice the final performance of any system will be strongly influenced by the quality of the detector used. As mentioned above, the HES spectrometer comes as standard with one of three standard detectors:

- HES 1000 An uncooled CMOS device
  - QE ~ 40 %; Read Noise = 7 RMS Dark noise = 0.1 count/sec/pix
- HES 2000 IVAC Cooled CCD
  - QE ~ 50 %; Read Noise = 5.6 RMS; Dark Noise =0.005 Counts/sec/pix
- HES 3000 IDUS 420 Cooled CCD
  - QE ~ 80 %; Read Noise = 3.8 RMS; Dark Noise =0.0003 Counts/sec/pix

These systems are compared to a mid range Czerny Turner system offered by a variety of manufacturers whose detector specifications are given below

QE ~ 80 %; Read Noise = 6 RMS Dark noise = 0.01 count/sec/pix

One of the main application areas for systems of this type is Raman spectrometry, thus the performance of these systems are compared with a spectrum of 100 pixels wide and signal levels of 100 and 1000 photons per second which are closer to those expected in typical measurements of diffuse sources. The resulting SNR for each of the detection options is given in Figure 7. The simulations assumed that the entire signal on the Czerny Turner device is captured in a line detector (1 pixel in vertical direction) and for each of the HES models the typical spread of the spectrum is taken into account. Thus in the case of the uncooled detector (pixel pitch < 4 µm) the signal is captured over 300 pixels in the vertical direction (this could be improved in bespoke systems).

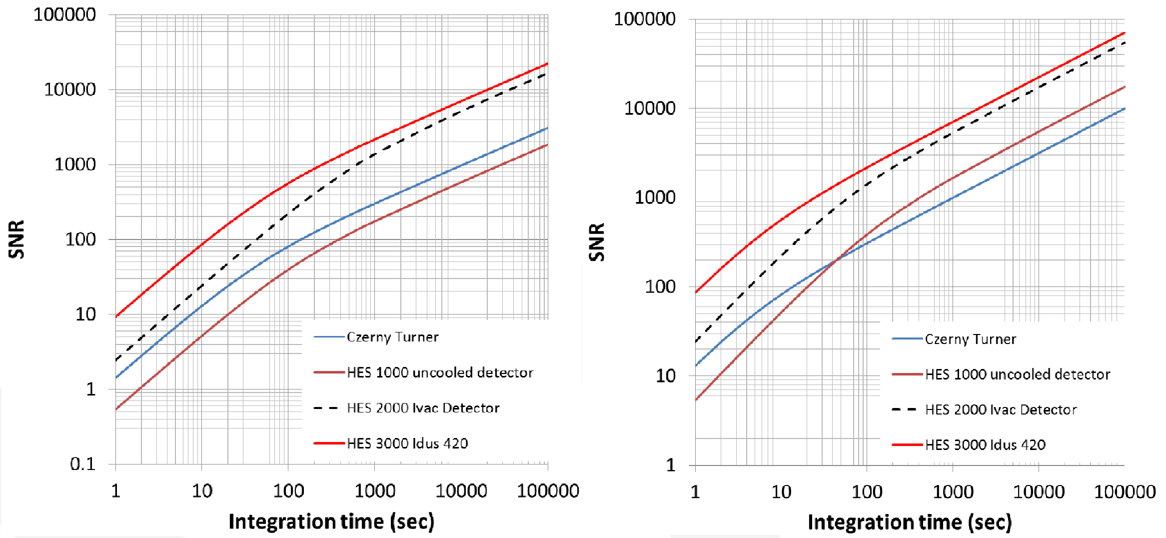


Figure 7 SNR comparison for of HES systems and Mid range commercially available Czerny Turner instrument taking account of detector specifications: LH image = 100 pixel per second observed ; RH image = 1000 pixels per second observe d. Dark Red line = HES 1000 spectrometer; Blue line = Czerny Turner performance; Dashed black line HES 2000 spectrometer; solid red line HES 3000 spectrometer.

As expected the bottom range HES 1000 spectrometer struggles against the Mid range Czerny Turner Instrument and the HES 2000 and HES 3000 models when the photon rates are 100 counts per second. This is due to the dominance of the detector noise and the lower overall performance of the detector compared to the example Czerny Turner. Once the count rate increases to 1000 ph/s, and more than 50,000 photons are collected, the superior throughput of the HES 1000 system allows it to observe a higher SNR than the Czerny Turner instrument. However, the mid-range and high performance HES spectrometer provide a SNR enhancement of greater than 2 for low integration times up to the shot limited case of 7 as the signal strength increases.

In the previous simulations very low signal rates have been considered of only 10 ph/s. When observing such low photon rates, uncooled CMOS sensors would always be limited by detector noise and would be very poorly suited for such measurements. With such low photon rates one may consider a bespoke HES or Czerny Turner instrument using an EMCCD

Common specifications for such a detector are as follows:

QE ~ 50 %; Read Noise = 0.7 RMS Dark noise = 0.001 count/sec/pix

The performance of a HES and a Czerny turner using an EMCCD is compared to the HES 2000 and HES 3000 models, with low photons levels of 10 and 100 photons per second. The spectrum is assumed to be 100 pixels wide in both cases.

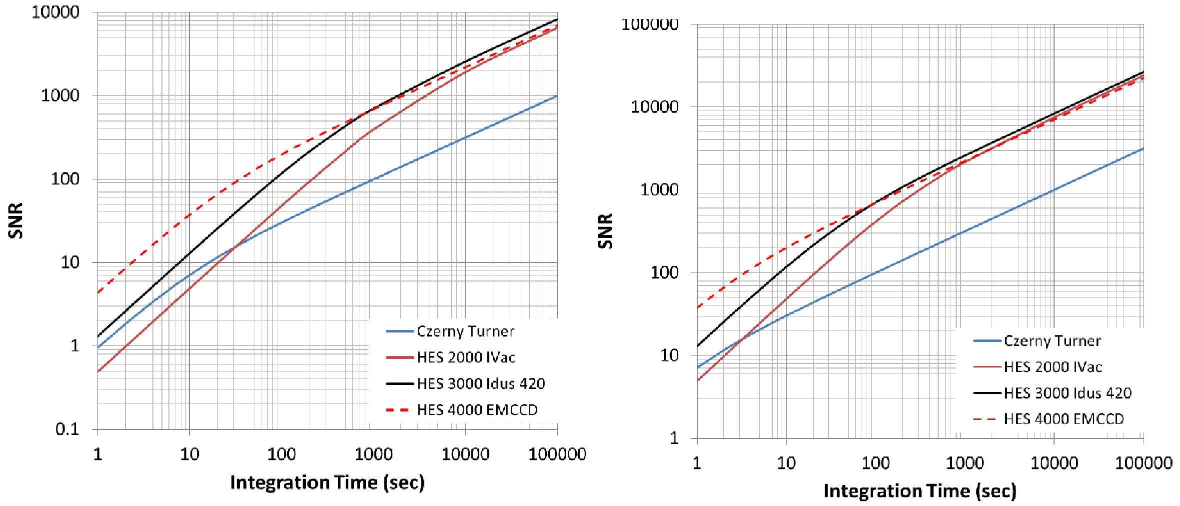


Figure 8 SNR comparison for of HES systems and mid-range commercially available Czerny Turner instrument taking account of detector specifications: LH image = 10 photons per second observed ; RH image = 1 photon per second observed. Dark Red line = HES 2000 spectrometer; Blue line = Czerny Turner performance; Dashed Black line HES 3000 spectrometer; red line HES 4000 spectrometer.

Figure 8 shows that the EMCCD model provides close to the shot noise limited performance even when the photon rate is 10 ph/s. Thus, the HES spectrometer enjoys a factor of between 5 to 7 enhancement in all the cases considered. The EMCCD does also significantly improve the performance of the Czerny Turner instrument. However the performance of the HES3000 is superior to the Czerny turner instrument in all cases and even provide a better SNR than the HES 4000 system once photons observed exceed ~ 10000. This is due to the higher QE offered by this instrument. These simulations show the importance of not only selecting the best spectrometer for a given task but also the detector must be carefully considered for the given application. The HES 2000 system which is a very price competitive system offers a competitive performance comparison to the Czerny Turner instrument, even when is uses an EMCCD, providing superior SNR once the signal exceeds 400 counts.

Table 2 presents a summary of the SNR returned for each of the options considered in this section at 1, 10 and 100 second respectively.

Table 2 Summary of SNR returned for the HES model instrument and Czerny Turner systems with different detectors

	HES 1000 (uncooled CMOS)	**HES 2000 (IVAC)**	**HES 3000 (IDUS 420)**	**HES 4000 (EMCCD)**	**Mid Range Czerny Turner**	**EMCCD Czerny Turner**
10 ph/ s 1 second	0.05	0.48	1.3	4.3	0.16	0.95
10 ph/ s 10 second	0.51	4.87	12.9	37.3	1.63	7.05
10 ph/ s 100second	3.97	47.59	116.5	196.4	14	30.01
100 ph/ s 1 second	0.53	4.9	12.8	37.5	1.64	7
100 ph/ s 10 second	5.2	47.9	116.8	199.2	14.7	30.13
100 ph/ s 100 second	39.6	411.2	703.2	696.9	84.2	99.5
1000 ph/ s 1 second	5.4	47.9	116.9	119	14.7	30.1
1000 ph/ s 10 second	51.4	413.3	703.9	698	85.6	99.5
1000 ph/ s 100 second	385.3	2186.6	2592	2232	309.9	316

CONCLUSIONS

The HES range of spectrometers have a significantly larger etendue or throughput, than covenantal dispersive systems. This makes them ideal for observing diffuse sources such as those required in transmission Raman measurements, and for integration into larger instruments. The devices are compact and cost effective, and can provide significant improvements in the SNR measured from a particular source.

The expected SNR returned by IS-Instruments High Étendue Spectrometer (HES) has been compared to that of a traditional Czerny Turner Spectrometer. The treatment presented takes account of both shot noise and detector induced factors. The treatment has been conducted initially assuming that both systems use the same detector to provide an indication of the performance of the optics alone. Secondly, the HES range of spectrometers have been compared directly to a mid-range, commercially available Czerny Turner Spectrometer taking account of the difference of the different detectors. These in turn are compared to the performance of a bespoke HES and Czerny Turner instrument using a top range EMCCD, offering near photon counting performance.

The analysis shows that the high throughput of the HES can provide up to a factor of 7 improvement on the SNR measured by the instrument when examining identical samples from diffuse sources. This is when the shot noise limits the performance and not detector effects. The HES system is more sensitive to detector noise in the low signal regime as the signal returned from any spectral line is analysed by the complete array detector. Thus, for very narrow spectral sources in isolation, the HES 2000 or HES 3000 range is recommended to gain the full SNR advantage.

The starting range, the HES 1000, is outperformed by a high quality, mid-range Czerny Turner instrument when the signal levels are low (<25000 counts). This is due to the noise inherent in the uncooled CMOS detector selected. This situation is reversed when the mid-range, HES 2000 is adopted. This provides up to a factor of 5 improvement in the SNR, even for modest signals. The HES 3000 range typically provides a factor of 7 improvement.

The multiplex advantage offered by the HES instruments further improves the performance of the instrument when broader with multiple spectral lines are examined. This makes the instrument ideal for applications such as Raman spectroscopy.

Finally, the HES performance was examined using an EMCCD and compared to a Czerny Turner system using the same state of the art detector, which offers near photon counting performance. In this combination the full advantages of the HES instruments are realised as detector noise effects are almost completely nullified.

It should be noted when a EMCCD is used for the Czerny Turner instrument that the HES 3000 model and once the counts exceed 400 the HES 2000 instrument still provide a superior SNR for diffuse sources, despite being significant lower in price.

In conclusion the analysis presented provides an overview of the strengths of weaknesses of both types of instruments and demonstrates the potential gains that gain be realised by the HES instrument range in applications such as Raman spectroscopy.