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ABERRATION CORRECTION IN THE BREWER SPECTROPHOTOMETER

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Abstract — The optical design of the Brewer Spectrophotometer has been optimised for measurements in the 300–320 nm wavelength range. An aberration resolution limit that is much less than the 0.6 nm FWHM (full width at half maximum) is achieved by using an Ebert–Fastie spectrometer design, modified by the inclusion tilted lens that optimises performance at 310 nm. The small contribution of the remaining aberration to the measured instrument function is critical to radiometric measurement quality. Ramifications of this design to the development of instrumentation with enhanced scanning abilities are discussed.

INTRODUCTION

The Brewer Spectrophotometer is used to perform both automated trace species quantification and radiometric measurements. Although these measurements are discussed elsewhere[1], the dual requirements of the Brewer necessitate a particular optical design. This work describes the design of the spectrometer within this instrument, and its rationale.

Trace species quantification requires rapid switching between a number of different, but precisely determined and repeatable, wavelengths. Accurate radiometric observations require that the instrument function be stable and repeatable across the entire scan region, and that the spectral pass-band be independent of the direction of incident radiation. The design chosen to satisfy these two different requirements is a modified Ebert–Fastie spectrometer.

A review of the Ebert–Fastie spectrometer is given by Fastie[2]. This paper addresses the need for modification of the Ebert–Fastie to the Brewer design for trace species measurement and radiometry. The importance of these design features is demonstrated by quantitatively expressing modelled performance of these systems in two examples. The quality of the observed spectra is critically dependent on the stability of this instrumentation.

EBERT-FASTIE DESIGN

Fastie[3] discusses the layout and details of the Ebert-Fastie spectrometer. Shown in Figure 1(a), this instrument uses a reflective plane grating as the dispersive element, and a single mirror to both collimate and focus the light. Using a single mirror makes alignment simpler than in a two-mirror design. Reflective optics allows the instrument to function well over a large wavelength range, and provides a system with a compact folded light path.

The conventional Ebert–Fastie spectrometer has a number of subtle design features. Coma induced in the image by the first mirror is partially compensated by the second mirror. In the symmetric case (where the grating is replaced by a plane mirror) the net coma of the system is zero.

Focus correction is achieved through the use of curved slits. Figure 2 illustrates how this slit shape produces good focus. If the main mirror surface is described as a section of a sphere of radius R, collimated light incident on this mirror will be focussed on the surface of a sphere with the same origin of radius R/2. If the image is placed on the surface of this focal sphere, the mirror will collimate the light, the grating will redirect this collimated light back to the mirror, and the mirror will focus the light again on the surface of the focal sphere. A linear slit cannot be focussed because a line will not lie on the surface of the focal sphere. The intersection between the flat plane of the slits and the focal sphere is a circle. When the arc of this circle describes the slits, they will be in focus throughout their entire length.

Curved slits also compensate for a natural curvature of spectral lines common to all grating spectrometers. Light from the centre of the slit will experience a slightly different dispersion than light at the ends of the slit. The relative positioning of the centre and ends of the curved slit will completely compensate for this effect.

BREWER DESIGN

The Brewer[4], shown for comparison in Figure 1(b), is a modified Ebert–Fastie spectrometer. The Brewer has three differences from the conventional Ebert–Fastie design:

(i) multiple straight exit slits are used;
(ii) the entrance and exit slits are displaced from the surface of the mirror's focal sphere, and
(iii) a transmissive 'correction lens' is placed between the entrance slit and the mirror.

The multiple exit slits facilitate rapid multiplexing between a number of precisely determined wavelengths. Measurements at these wavelengths are analysed to infer column densities of trace species such as ozone. The observation wavelength positions and bandwidths must be stable over time to ensure accurate measurements. Laser machined slit masks are used so that the spectral separation and shape of the slit pass-bands are highly repeatable between instruments. The absolute wavelength of the slits are set automatically by periodically positioning the grating with mercury emission lines.

The spectrometer is normally used in one of two modes. The first is a rapid switching between a few key wavelengths to determine trace species abundances; the second is a systematic scan through the UV spectrum (286.5 nm–363 nm) in 0.5 nm intervals. In the first mode, all slits must focus in the exit plane. In the second mode, the entire spectrum must remain in focus in the utilised exit slit(s) throughout the entire scan. The first

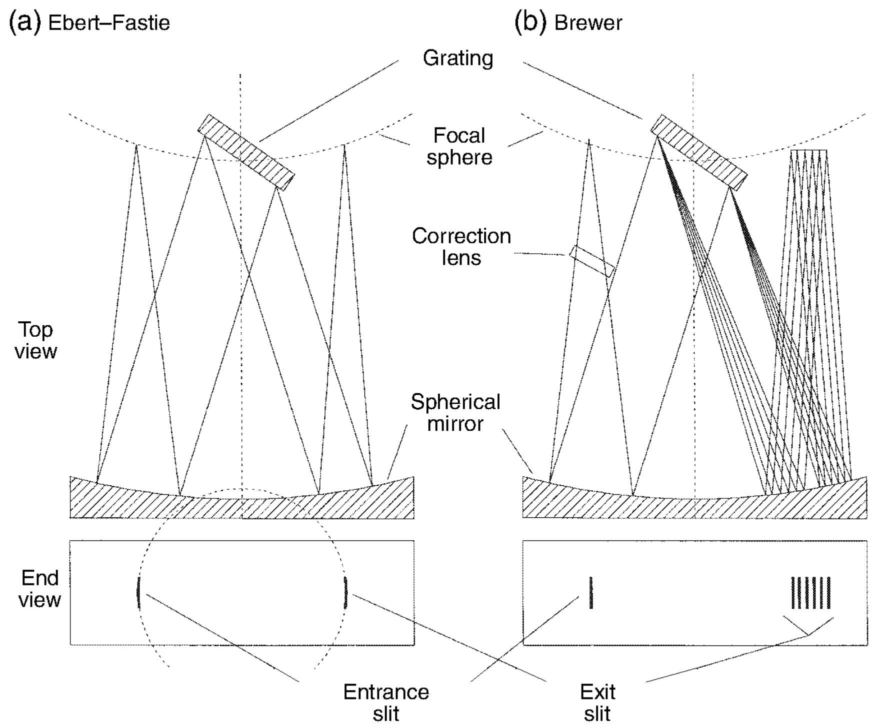

Figure 1. A comparison of the optical layouts of the Ebert–Fastie spectrometer (a), and the Brewer spectrometer (b). Slit heights are exaggerated to show the slit shape.

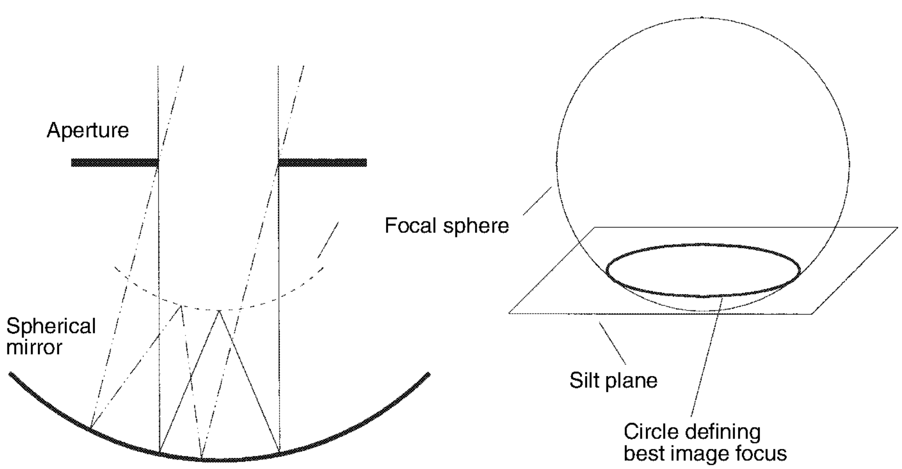

Figure 2. Collimated light will focus on the surface of a focal sphere, its position is dependent on the angle of the incoming light. The intersection of this focal sphere and the image plane is a circle.

of these objectives is satisfied by extending the distance from the mirror to entrance slit, and decreasing the distance from the mirror to the exit slit. This geometry is close enough to the optimal scan geometry that good focus is also maintained during the scan.

The correction lens used in the Brewer compensates for aberrations induced by the off-axis design. Details of the nature of these aberrations and how they are corrected are discussed in the next subsection.

Aberration correction details

An aberration free system would produce perfectly parallel light incident on the grating, and focus this light to a perfect image on the entrance slit. The off-axis design of the Ebert–Fastie spectrometer produces two optical aberrations that limit the performance of the system, coma and astigmatism.

Coma

Coma is the variation of the image magnification with respect to aperture. Although the coma induced during collimation is partially removed during focussing, the degree of removal is dependent on the symmetry of the system. Figure 3 shows that asymmetry is induced in the system by the grating. A consequence of the angle of incidence differing from the angle of diffraction is that dispersed light from the grating will have a beam cross section different from the incident light. This results in an imbalance in the amount of coma induced by the collimating and focussing processes. The operational angles for the Brewer grating induce significant net coma into the system. The spherical shape of the front surface and tilt of the lens act to minimise the net coma throughout the operational wavelengths of the system.

Astigmatism

Astigmatism is the difference in focal length of rays that are parallel and perpendicular to the instrument's axis of symmetry. The Brewer achieves a finer resolution by focussing differently from the classic Ebert–Fastie spectrometer. In the conventional system, the optics are focussed for minimum spot size. This is a compromise between focus in the dispersion direction (tangential), and the direction along the slit (saggital). In non-imaging applications, the resolution of the spectrometer is improved by adjusting for sharp focus in the tangential direction. With spherical optics, the price for this increase in performance is increased saggital blur. Instead of using purely spherical optics, the Brewer employs a cylindrical surface on the back surface of the correction lens to avoid this problem. The cylindrical surface minimises saggital blur when the tangential focus is optimised.

QUANTITATIVE RESULTS

The improvement in spectrograph performance over a conventional Ebert–Fastie system is illustrated in the following two examples. In the first example a conventional Ebert–Fastie design is compared with the Brewer design with a similar geometry to determine the relative contribution of various factors that limit spectrometer performance. A similar comparison holds true in the second example except that a different grating is used to achieve a greater spectral range. In both cases, the modifications show a large improvement in results.

Example 1 — Brewer design

The importance of the modifications to the Ebert–Fastie design becomes apparent in Table 1. Factors that contribute to the instrumental resolution are quantified for two specific cases. The first case is for an optimised Ebert–Fastie with design criteria similar to the Brewer, the second for the Brewer itself. Unless otherwise specified, the tangential blur obtained from ray trace results is multiplied by the dispersion to quantify the contribution in units that specify resolution. Note that these values are not additive; they are the maximum extents of smoothing kernels. Their values are useful in show-

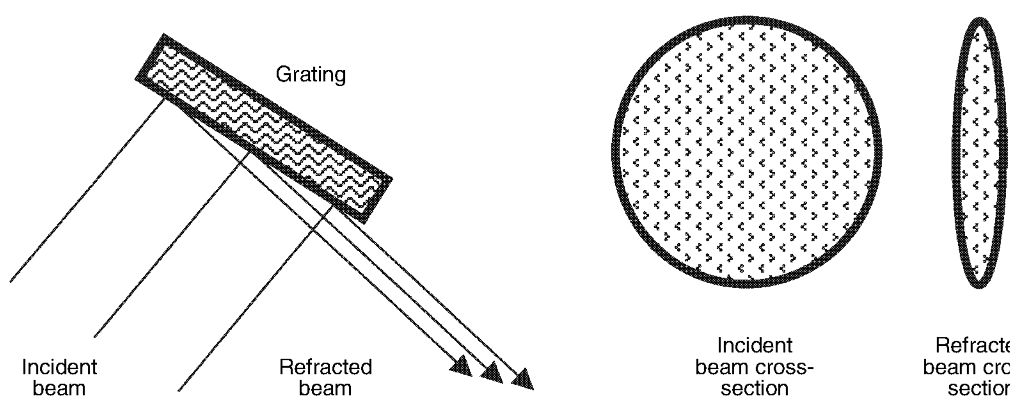

Figure 3. The grating compresses collimated light in the dispersion direction inducing a coma imbalance in the system.

ing the dominant factors that limit instrumental resolution.

The spread due to diffraction was determined from the formula for diffraction limited resolution:

$$\Delta\lambda/\lambda = n\ m$$

where $\Delta\lambda$ is the diffraction limited resolution, λ is the minimum wavelength, n is the diffraction order, and m is the number of grooves illuminated on the grating. In this situation we assume 70% of the grating grooves are effectively illuminated. The diffraction limited resolution is identical in both cases because the gratings and wavelengths are the same. The small value of this number in comparison to the others in the table shows that neither system is diffraction limited.

Temperature variability of the blur function was determined from the change in path length induced by thermal expansion/contraction of the spectrometer. A paraxial optical system of the same F# was used to calculate from the tangential blur, given the expansion coefficient of the optical bench and a ±25°C temperature change. This value was multiplied by the linear dispersion, then multiplied by two to account for the blur induced in the collimation and focussing processes. For the Brewer, grating and pushrod temperature coefficients[5] partially compensate for this effect, making this value an upper limit. The relatively small value of this factor means that both systems are relatively temperature invariant.

As mentioned in the description of the Ebert–Fastie system, considerable blur in the dispersion direction is induced by focussing to balance astigmatism. Because this is the dominant factor contributing to the system's resolution limit, the astigmatism contribution to the resolution is quantified from the total tangential blur.

This is very different in the case of the Brewer. The Brewer is focussed so that the contribution of the tangential blur due to astigmatism is very small. Instead, the significant factor affecting the blur is the variation in focus as the spectrograph is scanned in wavelength. This was quantified by determining the difference in blur between the optimal tangential focus and the true path lengths in the spectrometer. All wavelengths were used to determine the extremum of this difference, which was used to calculate the value in Table 1.

Table 1. A comparison of factors contributing to the resolution limit of two spectrometers employing high dispersion gratings.

Contributing factor	Ebert–Fastie design	Brewer design
Diffraction	0.003 nm	0.003 nm
Temperature focal variability	0.04 nm	0.04 nm
Field curvature and astigmatism	0.7 nm	0.2 nm
Coma	0.25 nm	0.02 nm
Spectral curvature	0 nm	0.01 nm

Coma was also determined in a similar way. For the Brewer, tangential blur was determined for ideal tangential focus, optimal correction lens angle, and at each wavelength. This residual was quite free of coma; spread in the dispersion direction was of a similar value to the diffraction limit. Values were then obtained in a similar way, but with the fixed correction lens angle used in the Brewer. Extremes of these differences were used to quantify the Brewer coma in Table 1. Ebert–Fastie coma was found through a similar process, except the second value was obtained without a correction lens. Care was taken in this case to remove astigmatic effects from the Ebert–Fastie model by optimising tangential focus.

As shown by Fastie, a properly curved slit has no wavelength variability along its length. The wavelength variability along a straight slit was obtained by taking twice the distance (accounting for entrance and exit slits) between a curved and a straight slit and multiplying by the dispersion. The range of this variation is called spectral curvature in Table 1.

Although the curved slits of the Ebert–Fastie provide a good focal compromise and less dispersion variability along the slit, the coma correction and optimal dispersive focus of the Brewer provide an overall smaller blur in the dispersion direction by a factor of three.

Example 2 — Enhanced design

In a recent feasibility study a Brewer modified to scan from 285 nm to 400 nm was modelled. The purpose of this study was to determine the expected size of the instrumental blur function. Once this was known, the resolution and stability of the instrument could be predicted for any given slit size.

The best way to achieve this was to use a coarser grating than the Brewer Mk III uses; the physical layout of the spectrometer makes it difficult to increase the angular motion of the grating. Although two possible gratings were considered, results are quoted obtained by using a grating that would provide one-third of the linear dispersion of the original grating.

The Brewer Mk III was chosen for modification due to its excellent out of band rejection capability and efficiency throughout the measurement range. This instrument was intended only to perform spectral scans, and hence only one exit slit was modelled (in the symmetric position to the entrance slit). Physically, a number of changes were made to the optical layout of the instrument:

(1) The neutral position of the grating made a smaller angle with the axis of symmetry.
(2) The physical widths of the slits were decreased by a factor of three.
(3) The correction lens was mounted at a smaller tilt.

(4) The distance between the main mirror and correction lens was modified.
(5) The distance between the main mirror and exit slit was changed.
(6) The curvature of the cylindrical surface of the correction lens was changed.

Once the proper operational angles of the grating were determined, the correction lens angle was changed to optimise coma correction. Because the grating was changed to a more symmetrical position, coma was less problematic and the correction lens required less tilt. The distance between the correction lens and the mirror was then adjusted to minimise focal length variation over the scan, and the optimal focal length was determined. As with the original Brewer instruments, the modified Brewer was adjusted to provide optimal tangential focus. The radius of curvature of the cylindrical surface on the correction lens was then optimised to correct for astigmatism.

The results of these changes are shown in Table 2. Again, the new design capabilities are displayed with the traditional Ebert–Fastie design to provide a baseline of comparison. As with the previous example, the Ebert–Fastie design used a similar optical geometry. The system employed symmetric slit to mirror distances, did not use a correction lens, and was focussed for minimum spot size.

Comparing Tables 1 and 2 shows that decreasing the grating groove density has a number of consequences. The reduced groove density of the grating increases the diffraction limit. Again this is significant only in showing that the system is not diffraction-limited. In general, although the blur-spot sizes were the same or smaller, the decreased linear dispersion amplified the results a factor of three when these results were expressed in wavelength. Temperature-induced expansion or contraction of the spectrometer will cause a significant change in focus. The coarser grating introduces less asymmetry into the system and allows a smaller range of scan angles. This means that the physical blur size from coma over the scan was much smaller, although this effect is countered by the decreased reduced dispersion. Finally, the changes do not affect the natural curvature of the spectral lines, effectively tripling their effect for straight slits.

Table 2. A comparison of factors contributing to the resolution limit of two spectrometers employing low dispersion gratings.

Contributing factor	Ebert–Fastie design	Enhanced design
Diffraction	0.006 nm	0.006 nm
Temperature focal variability	0.12 nm	0.12 nm
Field curvature and astigmatism	2.1 nm	0.12 nm
Coma	0.3 nm	0.03 nm
Spectral curvature	0 nm	0.03 nm

The comparison of the two designs in Table 2 indicates that the enhanced design has significant advantages over the Ebert–Fastie design in terms of optical aberration correction. It is possible to create a repeatable instrument with the Brewer's resolution employing an enhanced scanning range because the line shape is dominated by the slit width, not optical aberrations.

DISCUSSION — MEASUREMENT STABILITY

The stability of a radiometric instrument is critically dependent on its instrument function. If the resolution of the instrument changes, it will have an unpredictable response to different types of spectral features. Figure 4 illustrates this point for the two extremes in spectra. In this example, the response to a line source and continuum are compared when the full width at half maximum (FWHM) doubles. The response to a spectral line is doubled because the entrance slit is twice as large and all of this light will exit the double-sized exit slit. The response to a continuum is quadrupled because the entrance slit is twice as large, and the exit slit samples twice the bandwidth of spectrum.

Another way of viewing this problem is in terms of units. A single spectral line has an intensity that is described as a photon flux. A spectral continuum has an intensity that is described as a photon flux per unit wavelength. Thus, it becomes obvious that spectra taken at two different resolutions have different response ratios to the same continuum and line features.

The spectrum UV radiometers read is a combination of continuum and line spectra. Consequently, it is important to have a consistent instrument function across the scan in order to interpret and compare this data properly.

The overall resolution of the spectrometer is determined by the geometry of the entrance slit, exit slit, and the spectral blur function. Although the degree of blur is a function of the scan position, the slit size varies slowly and predictably. Thus, if the size of the slits is much larger than the blur, the line shape (hence resolution) of the spectrograph is predictable through the scan. On the other hand, if the blur function is larger than the slit size, the spectrometer instrument function will be quite variable.

The geometric slit function of the Brewer is 0.55 nm wide. When this slit function is convolved with the instrumental blur function, there is very little change in line shape. The consistency of its instrument function makes it ideal for radiometric applications.

The coma component of the blur essentially produces a wavelength shift of the slit function dependent on the entrance direction of the radiation. Thus, different parts of the field of view result in measurements at different wavelengths. This causes fundamental wavelength uncertainty unless the source radiance distribution is known and constant. A common outcome of coma aberration in spectrometers is that the wavelength calibrations depend significantly on the precise position of the spectral lamp being used for the calibration.

CONCLUSION

The Brewer spectrometer is designed specifically to perform radiometric scans in the UV, and to determine the column abundance of trace atmospheric species. For this reason, it was necessary to incorporate several design modifications from the traditional Ebert–Fastie spectrometer.

Multiple exit slits allow fast and accurate measurements of trace species. Asymmetric placement of the entrance and exit slits gives a focal length that is invariant with respect to exit slit and grating angle. A torroidal lens provides both coma and astigmatism correction. By focussing this system for minimal tangential blur, a resolution limit of roughly a factor of three can be achieved over the traditional Ebert-Fastie spectrometer.

The relatively small size of this blur function in comparison to the slit width means that the Brewer instrument function is very repeatable and that there is very little variation in wavelength over the field of view. These factors are critical to accurate radiometric measurements.

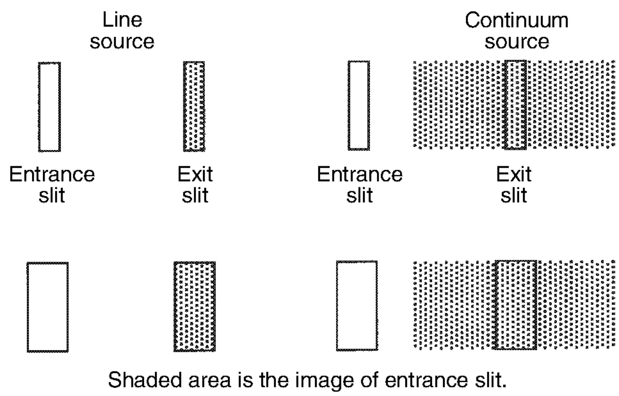

Figure 4. The response of a spectrometer is linearly dependent on the resolution in the case of a line source; quadratically dependent in the case of a continuum source.

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