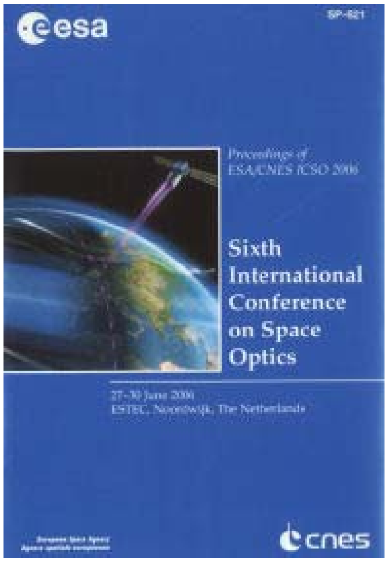

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PROBING THE HERMEAN EXOSPHERE BY ULTRAVIOLET SPECTROSCOPY (PHEBUS): OPTICAL SIMULATION OF AN ULTRAVIOLET SPECTROMETER

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ABSTRACT

PHEBUS (Probing of Hermean Exosphere by Ultraviolet Spectroscopy) consists of an ultraviolet spectrometer for the MPO (Mercury Planetary Orbiter) of the Bepi-Colombo Mission.

The goal of this instrument is to detect emission lines of Mercury exosphere in the bandwidth from 55 to 315 nm by recording full spectra. This instrument is made of an entrance mobile baffle, which is necessary to scan vertically the Mercury atmosphere, an off-axis mirror entrance, a slit, two gratings and two detectors. A few different designs, simulated by optical software, are analysed in this paper. They provide essential results as the instrument spectral resolution. Besides a radiometric model is established to observe the spectra we would obtain on the detectors.

1. PHEBUS INSTRUMENT OVERVIEW

1.1 BepiColombo mission

BepiColombo is devoted to the exploration of Mercury and its environment. The mission consists of two spacecrafts: the Mercury Planetary Orbiter (MPO) and the Mercury Magnetospheric Orbiter (MMO). PHEBUS instrument will be on MPO. PHEBUS is an international cooperation between France (Service d'Aéronomie, CNRS-IPSL), Russia (IKI) and Japan (JAXA).

The launch of the spacecraft is foreseen in 2013, and it will reach Mercury orbit in 2019.

1.2 PHEBUS scientific objectives

The atmosphere of Mercury is very tenuous, with a pressure of a fraction of picobar. It results from a complex interplay of the solar wind, its planetary magnetic field and its rocky surface. It is nearly non-collisional, and is highly variable with time and space, characterized by a global asymmetry between dayside and nightside and rapid temporal variations, possibly related to varying magnetospheric activity.

Five main categories of measurement objectives can be identified for PHEBUS:

1- To detect new species, including metallic ones (Si, Mg, Fe…), volatile atoms (C, N, S…), molecules and radicals (H2O, H2, OH, CO), noble gases (Ar, Ne), ions (He+, Na+, Mg+…), in addition to already detected species (Na, K, Ca, O, H, He) UV measurements from Mariner 10, and telescopic optical spectroscopy from Earth.

2- To measure an average exosphere (number densities of constituents, vertical structure), with as much as possible species monitored together, at different positions of Mercury around the Sun.

3- To measure sharp local and temporal variations of the exosphere content.

4- To search for albedo variations of Mercury's nightside surface, lighted by the interplanetary H Ly-α glow, at 121.6 nm, in order to exhibit possible signatures of surface ice layers (H2O, SO2, N2, CO2…) in high latitude polar craters, and any other signature of interest on the nightside.

5- Optionally, to search for UV reflectance signatures of Mercury surface in the 200-260 nm spectral range.

1.3 Instrument configuration

PHEBUS is a double spectrometer for the Extreme Ultra Violet (EUV) range (typical 55-155 nm) and the Far Ultra Violet (FUV) range (typical 145-315 nm) with an extension for some extra visible emission lines (calcium and potassium at 422nm and 404 nm respectively).

The instrument is composed of several subsystems, all included in a single box (Fig. 1). The front end consists of a stray-light rejection baffle and an off axis parabolic mirror allowing to scan of the Mercury exosphere thanks to a rotating mechanism. This movable mirror collects the light from the exosphere above the limb and directs it to the entrance slit. The parameters of the mirror were calculated so as to have a 170 mm working focal length focusing the beam on the slit, the beam folding angle being 100°. The beam is then spectrally spread by two holographic gratings and reaches the detectors.

The spectrum detection is based on the photon counting method and is realized using Micro Channel Plate

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(MCP) detectors with Resistive Anode Encoder (RAE). Typical photocathodes are CsI or KBr for the EUV range, CsTe for the FUV range. The size of the detectors' active area is 40x40 mm² equivalent to a matrix of 512x512 virtual pixels (spectral x spatial).

Furthermore calcium and potassium lines are selected by the FUV grating. These extra visible lines are monitored using Photomultiplier (PM) with bialkali also used in photon counting mode.

In order to prevent sensitivity losses which are critical in UV ranges, the number of optical components was reduced to have a minimum of reflections.

The main advantages of the MCP+RAE detectors are their very high sensitivity mainly due to a very low dark current. Thus photon counting is easily achievable on typical experiment temperature range (from -20°C to +40°C), avoiding mass and power expensive devices to cool the detectors. Seven orders of magnitude for the detection are then a typical value and offer the monitoring of a wide range of emission.

Moreover PHEBUS is a very flexible instrument due to a rotating scan mirror at the entrance. The instrument is then independent of the spacecraft on an observation point of view, avoiding spacecraft slew for specific pointing request. This scanning mirror is also very helpful to maintain the line-of-sight close to the limb during long integrations, to make the search and monitoring geometry less dependant on orbit and to extend the vertical range of scanning.

1.4 Optical specifications

The spectral performance of the instrument is specified by the Instrument Spectral Response Function (ISRF): it is the distribution of a monochromatic radiation along the spectral axis, as delivered by the instrument, before binning, i.e. before accumulation of slit image along the spatial axis. Thus, the following requirement applies to any profile across the spatial axis. The shape of the ISRF is described at two levels, by its Full Width at Half Maximum (FWHM), and its Full Width at 1% of the maximum (FW1%). For the EUV spectrometer, specified FWHM and FW1% are 1 nm and 2 nm respectively; for the FUV they are 1.5 nm and 3 nm. Full widths are applicable for the whole spectral range of the detectors. This ISRF shape has to be respected on the whole spatial axis of the slit image on the detector.

The spectrometers configuration has to manage with several constraints. The incident beam on the detector should be as perpendicular as possible because the detector efficiency is optimized for a normal incidence. The size of the total slit image must remain as small as possible along the spectral axis for spectral resolution of course, but also to constrain the spread along the spatial axis in order to keep a level of noise as low as possible.

Another constraint for the optical layout is that the more compact and the lighter the instrument is, the more appropriate it will be for space accommodation.

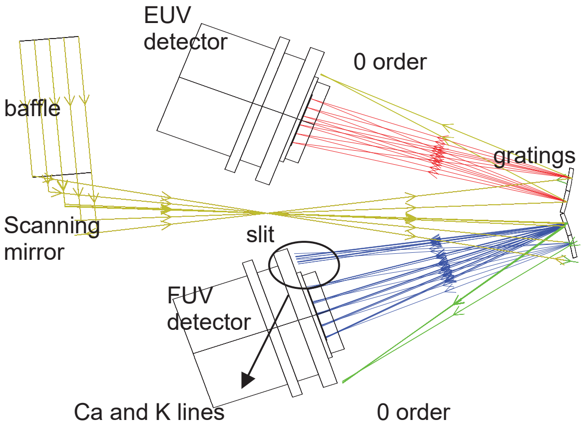

Fig. 1. Typical simulated configuration

2. OPTICAL SIMULATION

2.1 Optical models

To model the PHEBUS instrument, the first step is to determine the characteristics of the gratings which are the key components for the layout of the instrument. To simulate most of the optical elements of this instrument, we use the Zemax and Code V softwares.

Firstly, the simulations are computed with sequential ray-tracing method: a ray starts at the object surface, and then goes from one surface to the following in the order they are listed in. This method allows the design and the optimization of the system thanks to analysis tools such as 3D layout and spot diagrams.

We can model spherical or toroidal gratings, they are configured as holograms; the parameters of the gratings are the radii and the recording points.

Once these parameters are defined, we determine the position of the detectors.

The detectors are placed so as to have the best spectral resolution. The distance from the gratings to the detectors and the tilt of the detectors are optimised by the software on the whole spectral bandwidth. We have to verify whether the configuration is valid, in particular to check if the system is mechanically feasible. If not, we can tilt the grating to have a valid configuration.

By iterations on the grating parameters and on the position of the detector, we try to reach the resolution specified for each spectrometer.

We can determine the resolution of the system by using the spot diagram and geometric image analysis tools. The ray tracing method permits not only to determine the resolution but also the shape of the spots.

In order to have a more realistic model, we also have to determine if the ghosts introduced by grating diffraction orders, other than the useful one, will reach the detectors and if they will pollute the spectra. There are two kinds of pollution: ghosts introduced by one grating on the corresponding detector, and ghosts from one grating to the other spectrometer detector.

Another parameter is the size of the slit. We can study if we can make the slit larger to have more flux and if the specifications are still achieved. The nominal slit size corresponds to a 2° per 0.1° field of view.

The size of the instrument is a critical point since it is a space instrument. Thus different distances from the slit to the gratings and from the gratings to the detectors (called spectrometer arms) are studied. The nominal length is 200 mm.

Note that when we are simulating the gratings, we cannot take into account the manufacturing constraints due to a lack of knowledge concerning the manufacturing process. An industrial Call for Tender is on going to be sure of the feasibility of the system and to construct prototypes.

At last, we have to consider that all those simulations were calculated with ray tracing, and don't take into account such problems as scattering by the optics and the mechanical parts.

To determine the impact of those, we will have to simulate in non sequential mode, where rays are traced in physical order and not in the order objects are listed. This is essential to model stray light.

2.2 General results

Tab. 1. Tables of results for different configurations

EUV		FWHM (nm)	FW1% (nm)
Spherical gratings	*Min*	0.37	0.84
	Mean	**0.43**	**0.92**
	Max	0.58	1.20
Toroidal gratings	*Min*	0.36	0.73
	Mean	**0.46**	**0.97**
	Max	0.62	1.40
Toroidal gratings with short arms (110 mm)	*Min*	0.52	1.15
	Mean	**0.58**	**1.32**
	Max	0.78	1.88

FUV		FWHM (nm)	FW1% (nm)
Spherical gratings	*Min*	0.62	0.97
	Mean	**0.71**	**1.28**
	Max	0.97	1.77
Toroidal gratings	*Min*	0.62	0.97
	Mean	**0.70**	**1.40**
	Max	1.15	2.29
Toroidal gratings with short arms (110 mm)	*Min*	0.89	1.42
	Mean	**0.93**	**1.80**
	Max	1.24	2.66

Tab.1 presents the spectral performances of the different configurations calculated with our softwares. The FWHM and the FW1% are estimated for several wavelengths regularly spaced on the detector. EUV wavelengths are from 55 nm to 155 nm, by step of 5 nm. FUV wavelengths are from 145 nm to 315 nm, by step of 10 nm.

2.3 Nominal configuration detailed results

The chosen nominal configuration is the one with spherical gratings because toroidal was misadvised by industrials. On a spectral resolution point of view, the configuration with short arms was not selected, but it still remains as a back-up solution to propose a more compact instrument.

Fig. 2 presents the spherical gratings with nominal arms results for the EUV. Since the image of the slit does not spread on the total height along spatial axis of the detector sensitive area, only the central rows of the detectors are shown in Fig. 2. These images are quite efficient to discriminate good and bad resolutions. By summing columns, spectral profiles are obtained. Profiles vertical scale is graduated in relative energy, knowing that one emission line (i.e. one wavelength) contains a total energy of 1. Vertical scale is linear. Colour scale of detector response image is also linear. In order to estimate the resolution, couples of wavelength spaced of the specified FWHM are used. The couples used in the calculation are 55-56 nm, 80-81 nm, 105-106 nm, 130-131 nm, 154-155 nm for the EUV. The same calculations on FUV are realised with 145-146.5 nm, 190-191.5 nm, 230-231.5 nm, 270-271.5 nm, 313.5-315 nm wavelength couples. On graphs, wavelength increases from left to right.

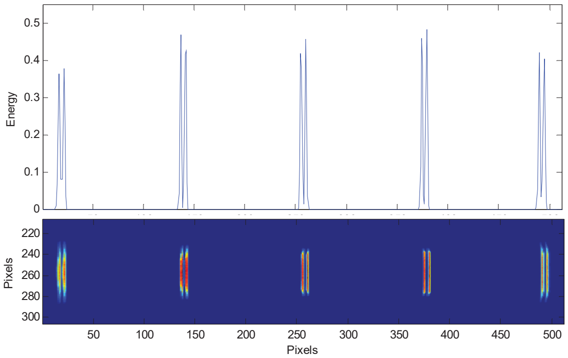

Fig. 2. Spherical EUV detector image and spectrum profile

3. RADIOMETRIC MODEL

The goal of this radiometric model is to explicit a precise description of the photometry of the instrument, as complete as possible, by taking into account a maximum of inputs and parameters.

3.1 Method

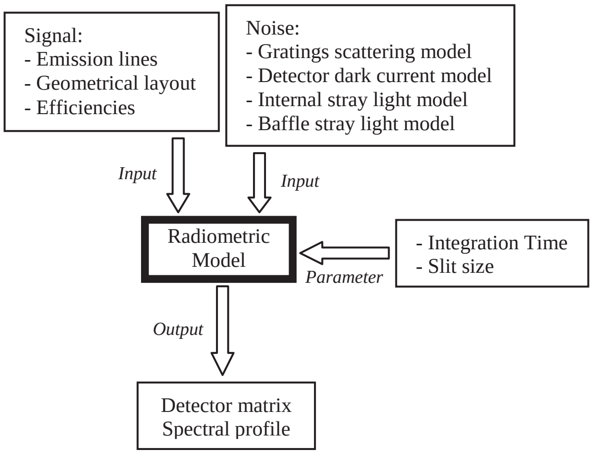

Fig. 3. Radiometric model method diagram

3.1.1 Signal inputs

First input is the light sources observed by PHEBUS: they are the emission lines coming from atoms in the Mercury exosphere. Each emission line is characterized by its wavelength in nanometres and its brightness in Rayleigh (1 Rayleigh is equal to 10^6 ph.s^{-1}.cm^{-2}).

Next input is a reference optical layout of the instrument, parameterized by many geometrical values such as pupil size, mirror focal length, slit size, gratings construction points, detectors positions... The chosen reference optical layout is the nominal solution, which contains spherical gratings and nominal length arms.

Last input concerns all the efficiencies aspects of the layout components: entrance mirror reflection coefficient, gratings efficiencies (at first and second orders), and detectors photocathodes quantum efficiencies (including window transmission for the FUV detector).

3.1.2 Noise inputs

Inputs concerning noise are more difficult to define. The first one is the detector dark current level, expressed in counts per second per square centimetre. Next input is the level of internal stray light inside the spectrometer part of the instrument. Another input is the baffle stray light noise model, which takes into account the performances of the entrance baffle and the solar flux reflected by Mercury's surface. Last input is a model for the scattering by the gratings surface.

3.1.3 Outputs

The radiometric model takes into account all the inputs to compute the response of the detectors as a matrix representing the number of counts per pixel. This matrix can be summed along columns (spatial axis) in order to obtain a spectral profile. Since the emission lines dynamic range is very wide, profiles are generally shown in log-scale. The emission lines are superimposed to this profile to identify the species.

3.1.4 Implementation

Two tools are used to perform the radiometric model: Matlab (numerical computation software) and Zemax (optical ray tracing software). Such an independent, polyvalent software as Matlab is required to perform general calculus that would be difficult to implement within Zemax.

A Matlab script calculates the expected count rates for each wavelength on each range (EUV and FUV), then writes several Zemax files (WAV format): due to Zemax limitation of 24 simultaneous wavelengths, these files contain the virtual central wavelength (with no photons) and 23 useful wavelengths, and there are as many files as needed to include all wavelengths of interest for the considered range. Matlab also calculates the total number of rays to trace with Zemax (see next paragraph) in order to simulate the right amount of photons reaching the detector. Each wavelength is attributed a weight, proportional to the number of photons it contains.

Additional WAV files are created for the superior orders of diffraction (gratings self-pollution only). By testing we have seen that Order 2 is sufficient.

Spectrometer configuration is opened in Zemax. For each WAV file, the Geometric Image Analysis tool is used in order to simulate the illumination of a pixelized detector. How many rays to trace? With the Geometric Image Analysis tool, we have to choose an extended source: a uniform source at least as large as the Field Of View of the instrument, i.e. a square source of width 2.5°. The total number of rays to trace is to be determined for this whole source towards the entrance pupil, then many rays will be launched, and only a few will propagate through the whole instrument to reach the detectors. This method is not very efficient in speed, but it is rather simple to implement and easy to control.

The Geometric Image Analysis tool outputs an image, which is a matrix containing the number of impacts (integer number of photons) on each pixel. Since the relative weight between all WAV files (including WAV files for superior orders of diffraction) is respected, the different images can be added with Matlab to obtain a full signal without any noise.

Matlab is now used to add imperfections and noise to the signal. Detector dark current and internal stray light noise are implemented as uniform noise on the whole detector. Baffle stray light noise is the result of the brightness of Mercury's surface out of guard angle and so decreased by the attenuation factor of the baffle, specified at 10^6. Scattering and diffraction by the gratings surfaces are not implemented yet because no precise information is available at the moment.

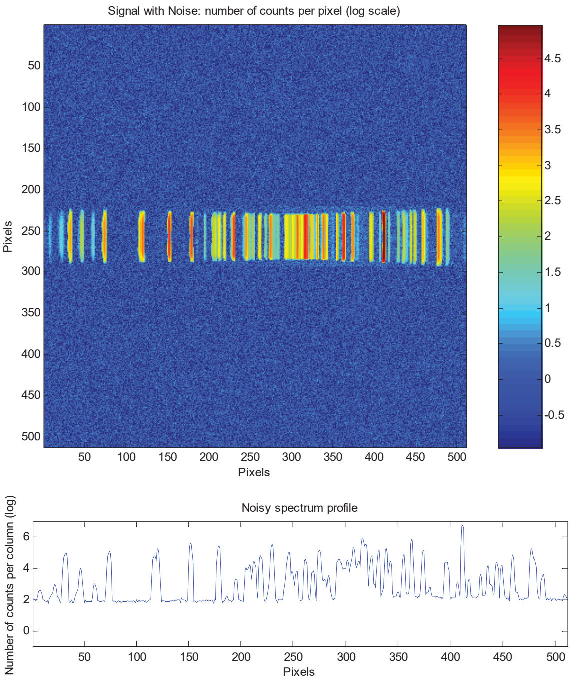

Fig. 4. A typical radiometric model output

3.2 Hypothesis of the radiometric description

3.2.1 Source

The expected brightness of the emission lines were estimated by NIST database. All the values are only rough estimations, since they could differ by a factor of 10, and they only represent an upper limit of the emission. The major detection issue is the very large dynamic range required (up to 7 decades) to observe as many weak lines as possible.

3.2.2 Collecting part

The entrance pupil defines the collecting area of the instrument. The slit, which is located at the mirror focus, defines the Field Of View. The product of these two values is the geometric extent, and it characterizes the quantity of light accepted by the instrument, thus the number of photons entering into the spectrometer part.

The flux collection is weighted by the reflection coefficient of the entrance mirror, which is nominally made of silicon carbide, with a SiC reflective coating.

3.2.3 Spectrometer part

The beam is divided into two distinct paths, one for each range. Thus only 50% of the light is lost when considering one path. Moreover, because of the physical gap between the two gratings, a small fraction of light is also lost. As a consequence, the photon flux that will be reflected towards the detector (all efficiencies issues apart) has to be multiplied by two factors: a factor of 0.5 for the spectral range separation, and another factor which is a little smaller than 1 for the gap.

Gratings absolute efficiency is the product of the relative efficiency by the reflectance of the material. The gratings are coated with Platinum. Relative efficiency is computed following equation (1), where a is the size of the grooves, λ is the wavelength, B is the blaze angle, α is the angle of incidence, and β is the angle of diffraction.

$$Eff_{Rel} = \mathrm{sinc}^2\left[\frac{a\cos B}{\lambda}\left(\sin(\alpha - B) + \sin(\beta - B)\right)\right] \quad (1)$$

3.2.4 Detectors

PHEBUS EUV and FUV detectors are composed of three elements: a UV sensitive photocathode of appropriate material, a Micro Channel Plate (MCP), and a resistive anode.

Each UV photon impacting on the photocathode has a chance to create a photoelectron that will be amplified by the MCP in order to generate a cascade of electrons. This process is quantified by the Quantum Efficiency (QE) of the photocathode. This avalanche then impacts on the resistive anode, which is coupled to an encoder that measures the impact position on the anode with a 9 digits depth. It "simulates" 512 by 512 virtual pixels. The value associated to the concerned pixel is incremented by one count.

The two spectral ranges use different photocathodes: KBr or CsI for EUV detector, CsTe for FUV detector. Each photocathode has its own spectral QE. The FUV detector is protected behind an MgF_2 window with a certain spectral transmission whereas the EUV detector works without window to be sensitive below 100 nm.

3.2.5 Computation parameters

Different spectral profiles can be traced depending on some parameters.

The wavelength range can be either EUV or FUV.

The integration time can be chosen as desired. Typical observations will last from 1 second up to 1 hour.

The number of pixels of the detector can be chosen. The number of pixels of the detector is nominally 512, but a reduction option down to 256 in order to save mass has been studied.

The width of the slit is an important parameter: in the case of a variable slit, the width of the slit could be reduced or increased from the nominal value. It intends to be a real advantage to improve spectral resolution (minimal slit) or on the contrary to increase light collection (maximal slit).

For the special case of the EUV, the choice of the photocathode is not frozen between KBr and CsI. The radiometric model can be computed for these two photocathodes.

3.3 Model results

We present here samples of results for a given representative wavelength range: from 180 up to 235 nm, which contains isolated lines, very close lines, and weak lines (isolated or not). Fig. 5, 6 and 7 compares the results for different slit sizes.

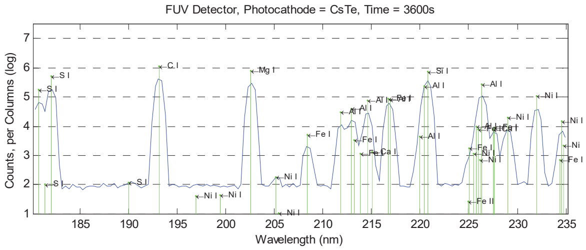

Fig. 5. Spectrum profile with a slit of 283 μm (nominal)

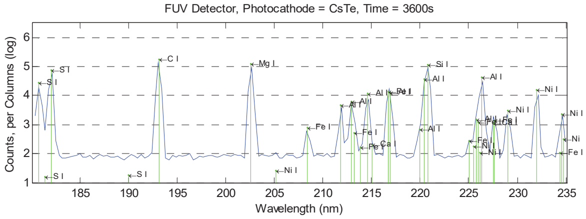

Fig. 6. Spectrum profile with a slit of 43 μm

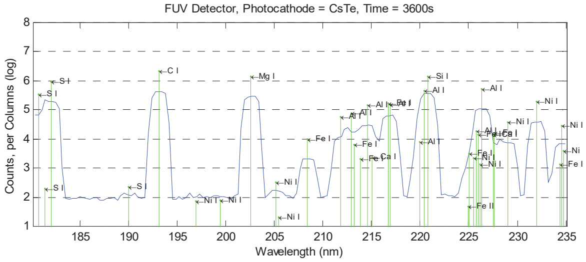

Fig. 7 Spectrum profile with a slit of 523 μm

For the EUV range with 1 hour of integration time, the expected species are: CO, He I, O I, H I, C I, N I, S I, S II, H_2, listed by decreasing brightness. The minimum detectable brightness is about 0.1 Rayleigh.

For the FUV range with 1 hour of integration time, the expected species are: Mg I, Si I, Na I, C I, Fe I,S I, Al I, CO, H I, Ni I, Mg II, O I, Ca I, H_2, Li I. The minimum detectable brightness is about 0.2 Rayleigh.

Some lines would require at least tens of hours or integration time to become visible.

Several lines are mixed with others and remain hidden although they are bright enough to be detected if isolated. For those lines, only a subtraction method can retrieve the line's count rate.

An interesting point is the Hydrogen Lyman-α (H I) visible on both detector, at first order on EUV and at second order on FUV.

The CO line at 151 nm is common to the two ranges (at the first order) and will certainly be a reference to cross-calibrate the two spectrometers.

3.4 Model limits

The current radiometric model presents some limits. The most important limitation is the uncertainties about the expected emission lines. All the efficiencies of optical components are estimated based on tabulated data found in specialized literature. They might not be exactly applicable to our components, which will need to be tested precisely. All noise and stray light levels are not well known at the moment. The current implementations are only estimations based on simplified hypothesis. Scattering and diffraction by the gratings still need to be taken into account.

4. CONCLUSION

The radiometric model based on the optimized optical design is indeed an essential tool in a scientific point of view. It will help anticipating the observations around Mercury and foreseeing which lines will be detected.

The model is also a very useful tool in a technical point of view, since it can help making technological choices, such as the kind of photocathode for the EUV detector.

It also permits to evaluate easily the impact of small changes at system level onto the instrument performances.

This model is expected to be refined with effective measurements on the real components, and also with in-flight calibrations. The goal is to describe a full radiometric model of the instrument applicable during scientific observations around Mercury.