X-shooter Physical Model

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ABSTRACT

We have developed a physical model of the VLT 2nd generation instrument X-shooter for use in wavelength calibration. We describe here the model concept, its use during the development of the data reduction software and the initial alignment of the spectrograph in the laboratory and the optimisation of the model to fit early laboratory data.

Keywords: Spectroscopy, Wavelength Calibration, Instrument Modelling

1. INTRODUCTION

X-shooter is a single target spectrograph for the Cassegrain focus of one of the VLT UTs covering in a single exposure the spectral range from the UV to the K band (320 -2500 nm). It is designed to maximize the sensitivity in this spectral range by splitting the incoming light into three arms (UVB, VIS and NIR) with optimized optics, coatings, dispersive elements and detectors, operating at intermediate resolutions (R=4000-14000). Each of the three arms constitutes an Echelle spectrograph with cross dispersion achieved through a prism (or multiple prisms in the case of NIR) in double pass and principle dispersion via a diffraction grating. X-shooter is currently undergoing subsystem assembly at ESO HQ in Garching and commissioning is scheduled for autumn 2008.

Traditionally the wavelength calibration of spectrographs relies upon an empirical approach. An exposure of a source, usually an emission lamp, with clear, laboratory-calibrated features, is obtained. The location of features on this wavecal exposure are then matched to the catalogued wavelengths of the source, and a low order polynomial is fitted to the data points to provide an empirical relation between positions on the detector and wavelengths. A meaningful polynomial fit will require a sufficient density of useful lines distributed over the wavelength range of interest. Since such an empirical polynomial fit has zero predictive value outside the range defined by data points, a lack of calibration lines at the limits of the wavelength ranges and detector boundaries can be particularly critical.

We replace this empirical method of wavelength calibration by using our physical understanding of the instrument. We know from the design process that even sophisticated spectrographs can be accurately represented[1,2] as a series of matrix transformations. The X-shooter optical model has a model kernel that is a fast, simplified ray trace code. The speed with which the streamlined model can be evaluated makes it suitable for iterative evaluation for many different wavelengths and slit positions. Most importantly, parameters describing the configuration of the optical components can be optimized using the Monte-Carlo type "Adaptive Simulated Annealing" technique[3,4] so long as appropriate calibration data is available. Consequently we are able to fit the dispersion solution with a set of physically meaningful parameters.

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Besides providing a robust physical basis to the wavelength calibration, this approach enables us to investigate problems such as flexure, support the development of the data reduction software (DRS) by providing simulated 2D data, provide preview data for astronomical observations (see Bristow et al[7]).

This approach has already been successfully applied to STIS[9,10] and CRIRES[11] , here we describe the almost completed implementation for X-shooter.

2. THE X-SHOOTER PHYSICAL MODEL

Following the prescription of Ballester & Rosa (1997)[1] , the core of the X-Shooter physical model is a series of matrix transformations, each representing an optical surface in the spectrograph as specified in the detailed Zemax optical design[6] . This enables determination of the location at which a ray of given wavelength and entrance slit position intersects the detector plane. The matrix transformations embody the tips and tilts of the optical components. For example, let M_E be the matrix representation of the order m transformation performed by an Echelle grating with constant σ_E at off-blaze angle θ, then:

$$M_E = \begin{pmatrix} 1 & 0 & 0 & 0 \\ m/\sigma_E & -\cos\theta & 0 & \sin\theta \\ 0 & 0 & 1 & 0 \\ 0 & \sin\theta & 0 & \cos\theta \end{pmatrix}$$

This operates on a 4D vector with components (λ, x, y, z) representing a ray of wavelength λ. Here θ and σ_E are amongst the physical model parameters for this instrument.

The optical layout of the x-shooter UVB arm is shown in figure 1 (reproduced from the X-shooter Optical Design Report[6]). The UVB and VIS arms of the X-shooter spectrograph are very similar in design and can be described by the same set of matrix transformations, they simply require distinct parameter sets. The NIR arm is also very similar, having just two additional cross-dispersion prisms, therefore we are able to use a slightly adjusted model kernel and parameter set that includes the additional prism transformations and appropriate parameters. The parameter sets for the three arms can be summarised as follows:

- Entrance slit & collimator
    - Relative position and orientation of the slit
    - Focal length of collimator
- Cross-disperser Prism(s)
    - Orientation of entrance surface
    - Orientation of exit surface
    - Temperature
    - Refractive index (*not* a parameter but computed from reference data as a function of wavelength and temperature (see below)
- Reflection grating
    - Orientation
    - Grating constant
- Camera and detector array
    - Focal length of focusing optics
    - Orientation of detector
    - Relative position of detector
    - Dimensions of pixel grid

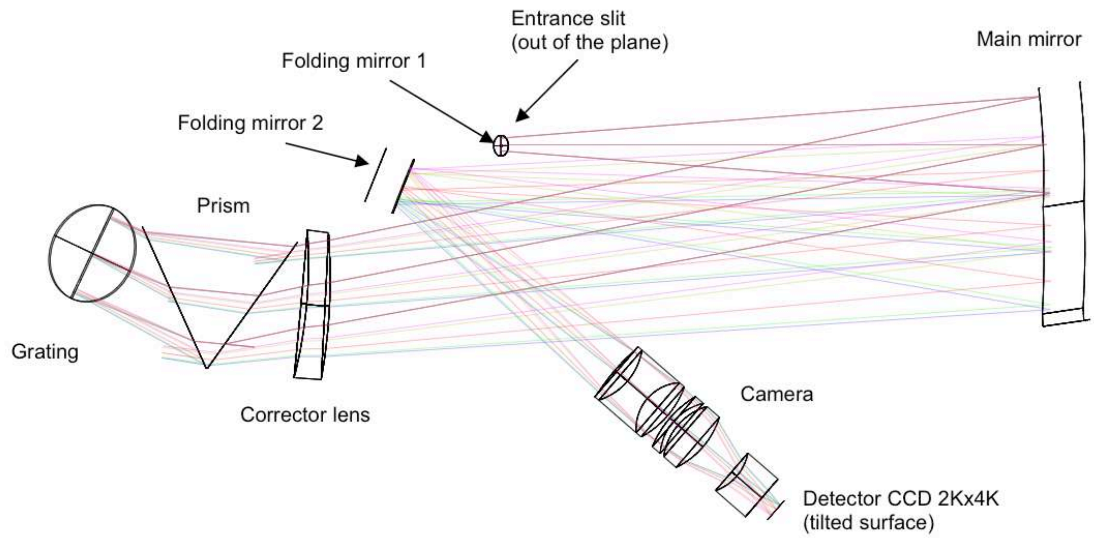


Figure 1. The optical layout of the X-shooter UVB arm, reproduced from the X-shooter Optical Design Report[6] . The VIS arm is qualitatively the same whilst the NIR arm is similar but has two additional cross-disperser prisms.

Hence there is a complete set of parameters that describe the passage of a photon through the spectrograph. These parameters are physical quantities (angles, distances, temperatures etc.) and describe the actual status of components. They can be adjusted at any time to match the observed behaviour of the instrument or to predict the effects of tilting/modifying a component.

Though based upon the optical design, this model is not intended as a substitute for the full-fledged optical Zemax model developed by the designers. However, it is sufficient for accurate wavelength calibration. Moreover this streamlined description of the optics makes it suitable for iterative use such as generating synthetic exposures and optimising the parameter set (see below).

The refractive materials used by X-shooter for cross-dispersion have refractive indices that are a function of wavelength and temperature. This dependence cannot easily be described by parameters that can be solved for with the iterative algorithm (described below) used to determine the other model parameters. However, we have obtained high quality laboratory measurements of the refractive indices of the materials involved[12] .

3. FITTING THE PHYSICAL MODEL TO REALITY.

The initial values for the model parameters that were used during development come directly from the optical design. Inevitably, at the pixel level, the real instrument differs in behaviour from the optical design and we need to fit the model parameter set to match reality.

We require a comprehensive and uniform set of robustly identified calibration features from dedicated calibration exposures. We then iteratively call the core model function for the identified calibration wavelengths, comparing the results of each iteration to the centroids for these wavelengths as measured in the calibration data. We employ the Taygeta[5] implementation of the simulated annealing technique[3,4] to continually adjust *all* of the model parameters until the best match between predicted and measured centroids is found. Figure 2 is a schematic representation of this procedure.

We use pinhole exposures (X-shooter is equipped with single and nine pinhole masks) of Thorium Argon hollow cathode lamps (in all three spectrograph arms) to acquire wavelength calibration data suitable for optimising the

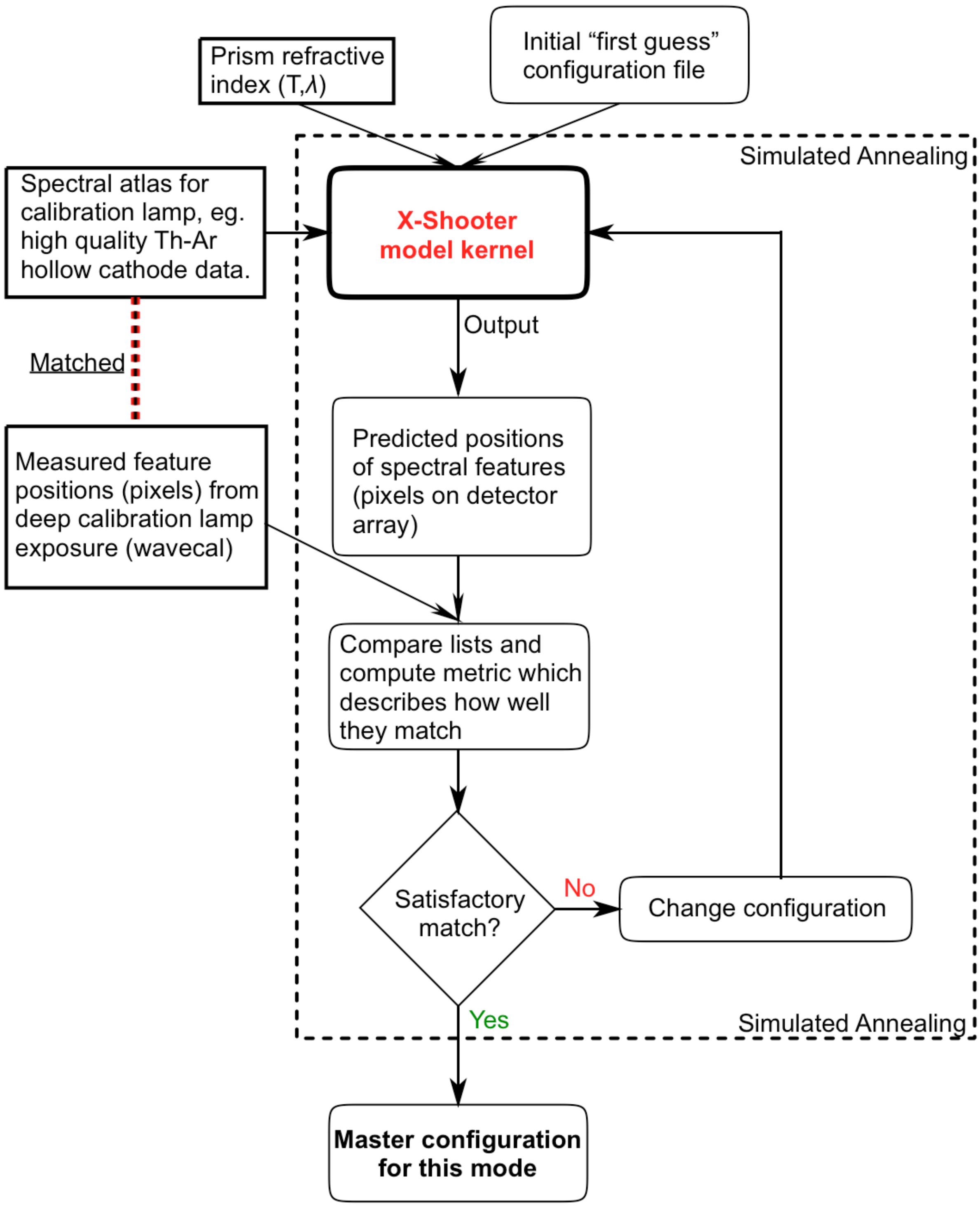


Figure 2. The optimisation process for the X-shooter physical model.

Table 1. Residuals. Here x is the cross dispersion co-ordinate and y is the dispersion co-ordinate. These residuals apply across the wavelength range of each spectrograph and along the length of the entrance slit. At the time of writing the physical model parameters for the NIR arm are currently being fit to the data.

	UVB	VIS	NIR
Δx (pix)	0.08	0.45	-
Δy (pix)	0.12	0.08	-
Δy (nm)	~0.001	~0.001	-
Max(x) (pix)	0.5	1.6	-
Max(y) (pix)	0.75	0.4	-
Max(y) (nm)	~0.0075	~0.006	-

model parameter set. The difficult task is the initial identification of calibration features *, since the optimisation process is sensitive to false matches. We are developing a technique that uses the model to derive customised line catalogues containing only calibration features that will be well isolated in X-shooter exposures[8] . This will enable us to simply search for expected features within an expected search box and be confident that we will not find false matches. For large search boxe sizes there is often a scarcity of such isolated lines, however one advantage of the physical model based approach is that it requires fewer data points in order to optimise the parameter set than is usually the case for the classical polynomial approach and there is no minimum number of feautures per order as is usually the case for polynomials that are fit independently to each order.

In this way we have been able to fit the VIS physical model parameter achieving the residuals (discrepancy between measured and model predicted locations for calibration features) given in table 1. Figure 3 shows a section of a real and (physical model) simulated VIS nine pinhole Th-Ar exposure.

Such a comprehensive optimisation of the model parameter set is only required when the instrument is first assembled or after a major hardware intervention or possibly after an earthquake. During routine operations we will monitor variations in the optimised parameter set, identify parameters whose values are not constant and support the automatic re-optimisation of these parameters in cases where a wavecal exposure, acquired at the same epoch as the science data, is available.

4. APPLICATION

4.1 Wavelength Calibration

The primary application of the physical model is driving the wavelength calibration. Once calibrated the model can be used to solve for the wavelength (and entrance slit position) that corresponds to the centre of any pixel on the detector.This information can be simply used to determine wavelength at any position along a conventionally extracted 1D spectrum. Alternatively the extraction itself could be driven by the physical model so that the flux in each pixel along the slit is associated with its specific wavelength and the wavelength scale re-sampled.

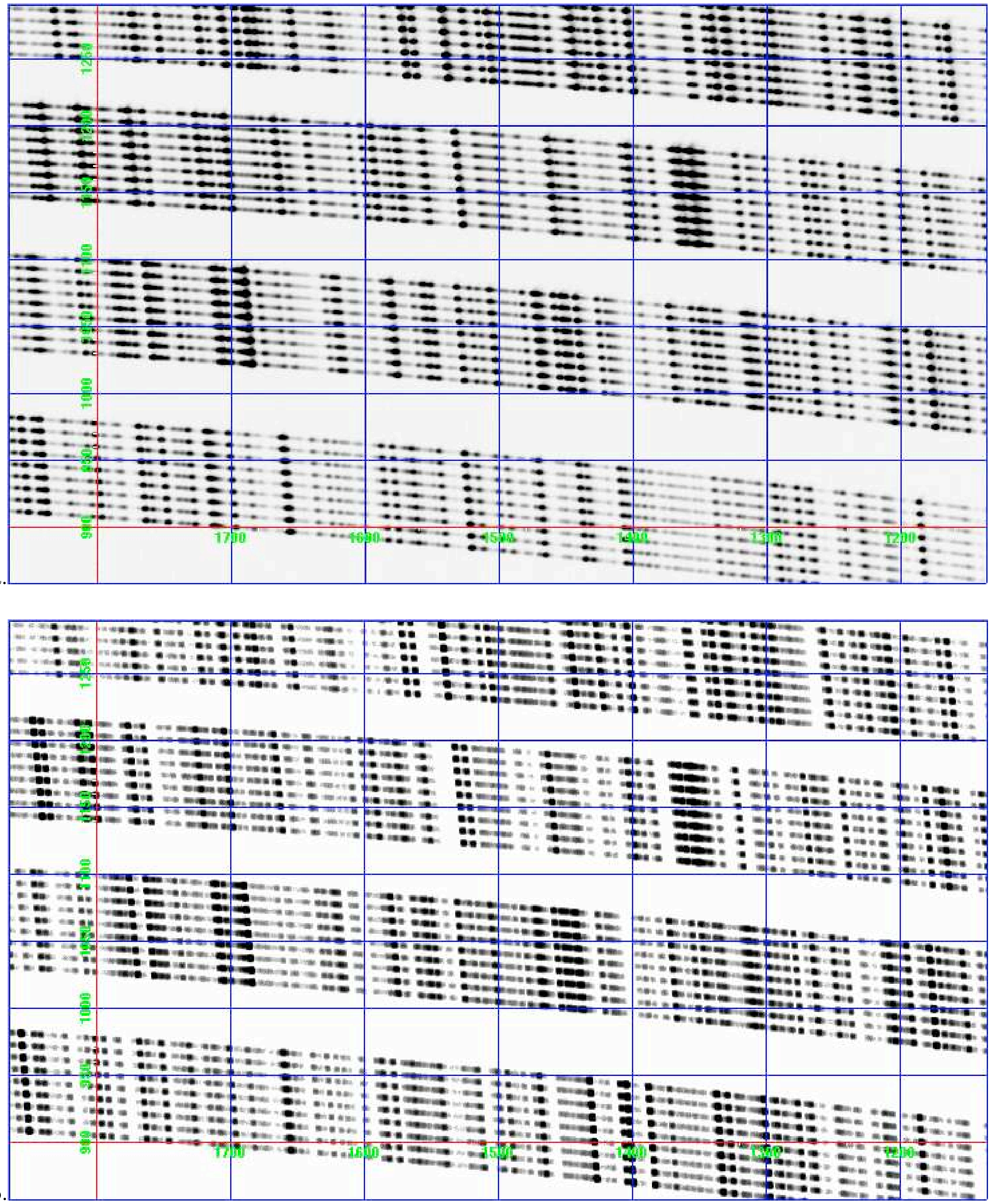
The following functionalities are available to the DRS:

Detector location For a given wavelength and entrance slit position the detector co-ordinates are returned. This is the simplest use of the physical model and is similar to the evaluation of a polynomial dispersion solution except that it returns a 2D position on the detector.

Order locus For all orders, the loci on the detector are returned.

Wavelength map For each pixel on the detector, the wavelength that would arrive at that pixel is returned.

*This is exactly the same problem that one faces when first determining the coefficients of a polynomial dispersion solution, except that the model parameters translated from the Zemax design provide a first guess.



a.

b.

Figure 3. a. Section of a real 9 pin hole mask, Th-Ar HCL exposure. b. Equivalent section of a physical model simulation based on the fitted model parameter set

Calibration feature centroids For a list of reference wavelengths and entrance slit positions, the detector co-ordinates are returned (essentially an iterative use of the first item above).

Spectral format The start, middle and end points of the orders in wavelength and detector space are returned (useful, for example, for initiating the limits between which spectral extraction should be performed.)

Refinement of physical model parameters Given an arc lamp observation and a corresponding line catalogue, the model parameters are automatically optimised to fit the data. This allows the physical model to react to small changes in the instrument behaviour during daily operations. Changes in the physical model parameters required to fit daily arc lamp exposures can be monitored in order to understand changes in the instrument and this data can be used for quality control.

The DRS can use these tools to drive the wavelength calibration and spectral extraction in the same way that they would use polynomial fits in the classical approach.

Each spectral order in a Cross dispersed Echelle spectrographs such as X-shooter has some overlap with neighbouring orders where unique wavelengths are imaged in both. This provides a useful test for the accuracy of the wavelength solution, since the wavelength assigned to a spectral feature should be the same regardless of which order and which part of the chip the flux was extracted from. Moreover this is a real challenge for empirical wavelength calibration where polynomial solutions have been independently fit to each order and often diverge at the extremes of the orders. Since the physical model is optimised simultaneously to data from all orders it is much better able to achieve a consistent fit in the order overlap regions. Figure 4 shows the excellent correspondence between the model wavelength solutions for neighbouring orders in UVB and VIS data (NIR results are not yet available).

Another potential problem for X-shooter calibration is the potential flexure within such a massive instrument at the Cassegrain focus. X-shooter will employ an automatic flexure compensation (AFC) system that uses short exposures of an arc lamp source obtained contemporaneously with every science exposure to achieve the required stability of the three spectrograph arms. This system corrects the beam entering the spectrograph slit, but flexure within the spectrographs themselves remains a problem. We hope to use the information in these exposures to optimise the model parameter set, providing a specific parameter set appropriate to the corresponding science exposure.The information in these exposures can be used to optimise the model parameter set. In this way we plan to assemble a database of optimised model parameter sets corresponding to different instrument orientations. Analysis of this database will reveal which of the model parameters are sensitive to changes in orientation and allow the dependence to be characterised. The effect of flexure in the dispersion solution can then be ameliorated by re-optimising the identified parameters using the AFC exposures. Furthermore, once the identified model parameters have been characterised as a function of instrument orientation parameters it will be possible to predict appropriate mean values for longer science exposures where the telescope tracks and the instrument orientation varies significantly.

4.2 Data Reduction Software Development

Since an early version of the X-shooter physical model was ready before the instrument was assembled, we were able to provide the team developing the DRS with synthetic data generated by the model before any real data was available. Clearly at that stage it had not yet been possible to optimise the physical model parameter set to the real instrument, but the approximate spectral formats were known from the design documents. We provided simulated 2D data for exposures of arc lamps and flat field lamps for a variety of entrance slit, pinhole mask and integral field unit configurations as well as the wavelength maps described above.

4.3 Instrument Alignment

The initial alignment of the spectrograph in the laboratory was aided by 2D simulated data of arc lamp exposures produced with the physical model. In addition the model was used to provide an accurate mapping of 2D offsets at the entrance slit to 2D vectors on the detector array.

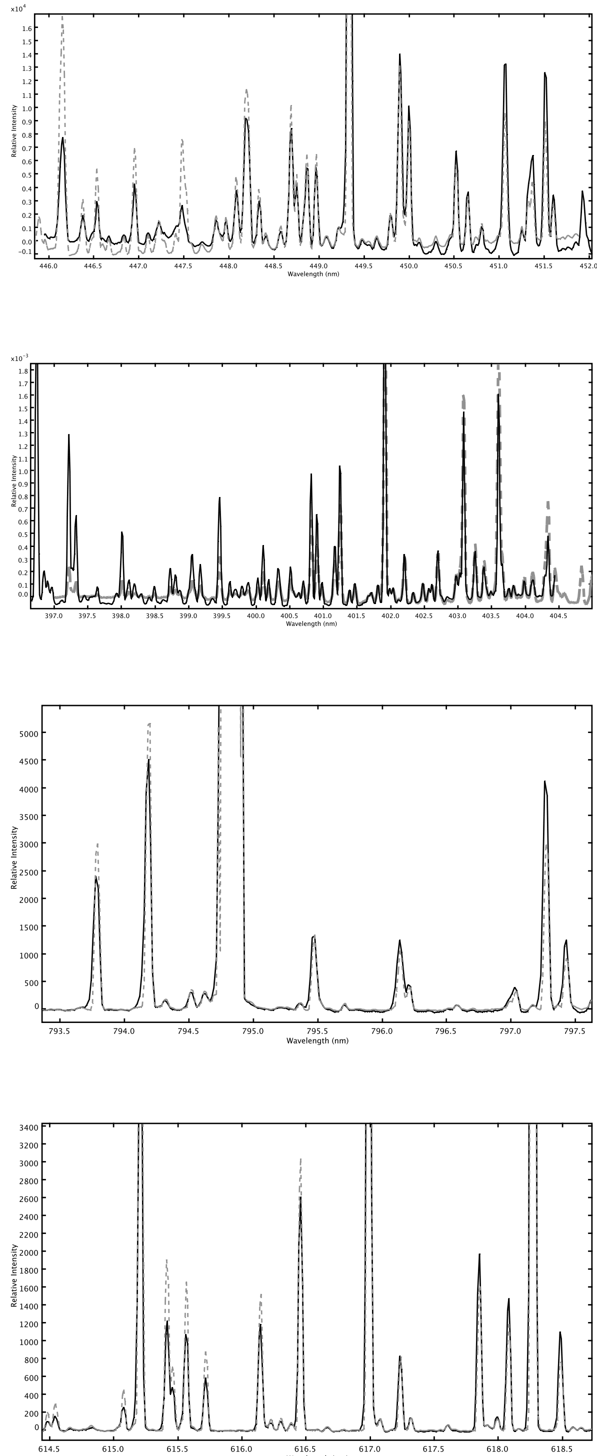


Figure 4. Example overlap regions, top to bottom: UVB orders 16 (dashed) and 17 (solid); UVB orders 18 (dashed) and 19 (solid); VIS orders 20 (dashed) and 21 (solid); VIS orders 26 (dashed) and 27 (solid). The difference in relative intensity for a given feature seen in two orders is due to the changing blaze function along the order. Systematic differences in the centroids of features detected in different orders is well below the centroid uncertainty caused by shot noise.

4.4 Previewing astronomical observations

A further potential application of the physical model is the possibility to provide detailed simulated 2D exposures given a synthetic or already measured source spectrum and a slit illumination pattern. This idea is discussed further by Bristow et al[7] .

5. SUMMARY

We have developed a streamlined physical model for X-shooter that comprises a model kernel and an associated set of parameters; each parameter has a clear physical meaning. In addition we have implemented the tools necessary to optimise the parameter set to match the actual configuration of the real instrument using dedicated calibration observations.

Once optimised, the physical model drives the wavelength calibration inside the data reduction pipeline. This is already an option for CRIRES and is being realised for X-shooter. We have also produced a suite of software to simulate 1D and 2D spectroscopic data using such models. These simulations have helped the initial alignment of the instrument in the laboratory and the development of the DRS and could potentially aid the planning of observations.

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