

Complete product design of an affordable spectrometer for hobbyist scientists



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# ABSTRACT

This report covers the complete design process of the IONICHEM Wave, an affordable spectrometer aimed at hobbyist scientists. The project includes aspects of industrial design, electronics, UI/UX design and optics. Through the project a spectrometer was developed which meets the needs of hobbyist users and fills a gap in the market.

# SECTION 1

Optical spectroscopy is the basis of many modern scientific analysis methods. It is a key part of today's laboratories, but high costs provide a barrier to entry to hobbyist scientists. Inexpensive instruments and kits are available, but their low quality and variability make obtaining consistent results difficult. This project aims to change that by providing a spectrometer with a balance of price and performance targeted at hobbyist scientists.

Visible light spectroscopy is used for various analyses in laboratories, particularly for measuring the concentration of known components of a sample. It is also used in industry for monitoring the thickness change of plastic sheets, and to gather information on the concentration of sugar, salt, proteins or acids in food production (Peiponen et al., 2009).



# SECTION 1.1

Currently available commercial spectrometers tend to be either excessively expensive and complex or of such low quality that they are impractical to use beyond basic qualitative analysis. The project's primary objective is to develop and prototype a budget spectrometer suitable for educational and general scientific purposes, with superior performance compared to currently available low-cost spectrometers on the market.

This project is a collaboration with IONICHEM, an analytical chemistry company based in East Sussex. The company has identified a need for low-cost visible light spectrometers aimed at the advanced hobbyist level with potential for classroom, field or even laboratory use.



## SECTION 1.2 METHODOLOGY

### **1.2.1 PROJECT GOALS**

- Bring higher-quality spectrometers to a hobbyist's price range IONICHEM set a target of £200-400
- Investigate the potential of modern low-cost cameras in spectroscopy
- Make a more accessible user interface than current options

## **1.2.2 COLLABORATIVE DEVELOPMENT**

As the project was a collaboration, regular check-ins were set up with the company. IONICHEM's Martin Teasdale represented the client in these meetings. Throughout the process, care was taken to get feedback from Martin to shape the development of the product. This meant demonstrating progress with hardware prototypes, and testing feasibility using Martin's home spectrometer setup.

## SECTION 1.3 DESIGN PROCESS

This project follows the double-diamond design process, with four stages: Discover, Define, Develop, Deliver. These stages roughly align with sections of the project, and so also define the structure of this report.

### DISCOVER

This stage is about gathering insight into the problem. Question what the focus of the project should be.

#### DEFINE

Focus on the important problems, and make sense of the possibilities identified in the discovery stage. Identify what is feasible and prioritise.

#### DEVELOP

Create, prototype, test and iterate on potential solutions. Improve and refine the idea with each iteration.

#### **DELIVER**

Focus on producing a practical, working solution and implement it.





# SPECTROMETER FUNCTIONALITY

An optical spectrometer splits light into its separate wavelengths and measures each wavelength's intensity. The intensities can be analysed to find information about the source or path of the light. A prism or diffraction grating splits the light into its spectrum. Different wavelengths of light are refracted or diffracted at different angles. Prisms do not spread the light as much as diffraction gratings, and they also reduce the intensity more (Kilkenny, 2009). Diffraction gratings are also smaller overall.

A beam of light enters a narrow slit at the front of the spectrometer, and is typically collimated with a lens. The narrow beam reflects off the diffraction grating, spreading the wavelengths apart. The light finally hits a photodetector array. At each point of the array a voltage proportional to the light intensity is output. These voltages are analysed to produce a spectrum. Variations use a transmission grating, which diffracts light passing through it rather than reflecting off it. To replace the collimating lens at the slit, some low-cost designs mount a focusing lens to the detector array. The key properties of a spectrometer are its range and resolution. A spectrometer's applications are determined by the range of wavelengths it can detect. For example, a spectrometer which can detect far-infrared wavelengths could be used for organic compound analysis, since different covalent bonds absorb specific IR wavelengths (Royal Society of Chemistry, 2017). A spectrometer's ability to distingish between different wavelengths is affected by its resolution. A low-resolution spectrometer may not be able to distinguish two sharp peaks close together.

### SECTION 2.2

# SPECTROSCOPY METHODS

Emission spectroscopy measures the wavelengths emitted by a light source. Excited electrons around an atom can drop to a lowerenergy state, producing atomic emission spectra. This process releases a photon. Electron energy level quantisation means that only specific wavelengths are emitted, characteristic of the atom. The atoms can be excited by an electric arc, a flame or a plasma (Harvey, 2013, p.201). The composition of the sample can be measured by comparing detected emission lines with those of known elements. The number of atoms is directly proportional to the intensity of the atomic emission line.

Absorption spectroscopy introduces a sample for analysis between the light source and the spectrometer. Some of the light is absorbed by the sample, and this can be characteristic of its composition. The light transmitted (passed) by the sample and that of a reference are compared. For each wavelength, the absorbance of the solution is calculated using the formula below, where *I* is the intensity of the sample's spectrum at that wavelength, and  $I_o$  is that of the reference.

$$A = -log_{10} \left(\frac{I}{I_0}\right)$$

The Beer-Lambert law relates the concentration of a part of the sample to its absorbance (Tissue, 1996). It is written as:

$$A = \varepsilon \times l \times c$$

Where *l* is the length of the light's path through the solution, and *c* is the concentration.  $\varepsilon$  is a wavelength-specific coefficient of absorptivity, and has units of  $M^{-1}cm^{-1}$ .

The amount of wavelength detail a spectrometer can resolve is difficult to quantify. One simple measure is to find the width of the sharpest peak the spectrometer can resolve. The standard way to do this is to measure the full width of the peak in nanometres at half its maximum intensity. This is called the FWHM (Full Width at Half Maximum).



Figure 2.2.1: Low-resolution spectrometer, fluorescent lamp spectrum.



Figure 2.2.1: Higher-resolution spectrometer, fluorescent lamp spectrum.

# SECTION 2.3 EXISTING PRODUCTS





#### **OCEAN OPTICS USB-650 RED TIDE**

Entry-level education spectrometer, which connects to Ocean Optics' extensive system of attachments. Based around a linear CCD. 350-1000 nm, 1nm/pixel, £900 (Spectrecology, 2016), (Ocean Optics, n.d.)

### ASEQ INSTRUMENTS LR1

Entry-level professional spectrometer based around a linear CCD sensor 300-1000 nm, 0.2 nm/pixel, £600 (ASEQ Instruments, 2015)



### THUNDER OPTICS MINI USB SPECTROMETER

Marketed as "the cheapest new USB spectrometer". Uses USB webcam instead of linear CCD.

400-850 nm, 1.5 nm/pixel, £75 (Thunder Optics, 2016)



### PUBLIC LAB DESKTOP SPECTROMETRY KIT 3.0

DIY Kit developed by community of hobbyists. USB webcam sensor. 400-700 nm, 3 nm/pixel, £35 (Public Lab, n.d.)



### SEKONIC C-700 SPECTROMASTER

Designed for lighting for photography and videography. Intuitive user interface on device. 380-780 nm, 1 nm/pixel, £1300 (Sekonic, 2014)

Many other spectrometers are available, but those shown are representative of the range of options on the market. Spectroscopy is such a mature field that there are very specific options available for all kinds of uses.

The Ocean Optics and ASEQ spectrometers command high prices due to their high quality. This puts them out of the price range of many hobbyists, and far from the target price set by IONICHEM. They demonstrate capabilities to aim for, particularly the Ocean Optics system of attachments, which has been built over decades and which makes them hugely versatile.

More affordable options such as the Thunder Optics spectrometer are low quality, and offer few benefits over a kit such as those made by Public Lab. These options are little more than curiosities, and would be difficult to attach to equipment for absorption measurements. The low price makes them worthwhile for some hobbyists. They highlight that a good balance of low price and high quality must be struck by this project.

The Sekonic C-700 is interesting in that it has a user interface built into the unit. This is similar to some higher-end laboratory spectrometers, but is very differently designed. Because it is designed for non-scientific users the interface is specialised for the few tasks required. Including a good user interface on the spectrometer could be a major differentiating factor from other low-end products.

# SECTION 2.4

Light sources are important for two different aspects of spectroscopy. The first is calibration. Without wavelength calibration, the intensity of each pixel is known, but not its wavelength. This can be useful for qualitative analysis (for example comparing a white LED with a halogen lamp), but absorption measurements are usually specified at a certain wavelength.

The wavelength of each pixel can be calibrated using a light source which outputs known wavelengths. Typically this is a vapour discharge lamp with very narrow intensity peaks. The locations of each peak on the detector (p in pixels) are related to the wavelength by a second-order polynomial (Ocean Optics, 2003).

$$\lambda_p = I + C_1 p + C_2 p^2$$

After the initial calibration, I,  $C_1$  and  $C_2$  should remain constant through the life of the spectrometer. Laser diodes have peaks of known wavelengths, but the peak is often wider than atomic emission peaks and may vary between lasers.

The light source is also critical for absorption spectroscopy. Ideally it would provide full intensity on the photodetector across the whole range of wavelengths. A lower intensity results in a lower signal-tonoise ratio. Many commercial spectrometers use deuterium, or xenon discharge lamps due to their wide band emission. For smaller or cheaper devices, a LED sources may be viable depending on the wavelengths being studied.

## SECTION 2.5 LIGHT SOURCE TESTING

Two main options were identified for the spectrometer's light source: incandescent lamps, and white LEDs. The properties of the light output of each was investigated using an Ocean Optics USB2000+ spectrometer. Incandescent lamps pass an electric current through a tungsten filament, and its resistance causes it to heat up. This creates a broad-spectrum light source (Figure 2.5.1), although lacking in blue light. A significant portion of its output is in the infrared region, which is potentially useful for expanding the spectrometer's range.

White LEDs use a blue light emitting diode covered with a yelloworange phosphor. This creates a light which looks white to human eyes, but which has a low intensity in the cyan region (Figure 2.5.1). This means that the area around 470-500 nm would have a low sensitivity.



Figure 2.5.1: Spectra of incandescent lamp and white LED. Note that visible wavelength range is 400-700 nm.

A combination of different wavelength LEDs was also considered. While wider than that of a laser diode, the spectral bandwidth of LEDs is still narrow. A FWHM of 13nm was measured for a green LED, resulting in very little overlap between the output of red, green and blue LEDs (Figure 2.5.2). Additional LEDs with intermediate wavelengths can be added to fill the gaps in the spectrum, but a roughly even output would require tens of LEDs, all focused into the same area.



Figure 2.5.2: Spectra of three coloured LEDs.

The more even spectrum of the incandescent lamp is ideal for absorption measurements. Sharp intensity peaks can make it difficult to distinguish signal from noise. The advantage of LEDs over incandescent lamps is the much higher efficiency, resulting in less heat production for more brightness (Walker, 2017). Additionally, LEDs are usually more directional, making it easier to direct their light output into a fibre optic. However, the limited bandwidth of LEDs is unfeasible to overcome and outweighs their advantages.

The characteristic orange light of incandescent lamps means that sensitivity is low in the blue region. The image sensor needs to adjust its exposure for the brightest area of the image: the longer wavelengths. The lower relative brightness of the shorter wavelengths





## SECTION 2.6 INDUSTRIAL REVIEW EVENING

The Industrial Review Evening on the 14th November 2017 offered an opportunity to discuss the spectrometer concept with design industry experts. The key feedback was that further understanding of the users was needed. In particular, this would allow targeting the product towards a specific niche, resulting in a more useful product in the time available for this project. The main research areas suggested were the user background, what they would use spectroscopy for, and their reasons for using it.

## SECTION 2.7 USER QUESTIONNAIRE

Some initial assumptions had been made about the target market. "Hobbyist scientists" can refer to amateur scientists, but also professionals who pursue it outside work. This was assumed to be primarily chemists, but also include biologists and physicists.

An additional market which was not investigated is teachers wishing to teach spectroscopy. Rodrigues et al. (2015) mention that spectroscopy "usually requires sophisticated and expensive equipment that is not normally affordable for schools", and highlight the need for low-cost options. The UK National Curriculum for A-level chemistry (GOV.UK, 2014) covers several spectroscopy methods "in analysis, including techniques for elucidation of structure". Visible light spectroscopy for quantifying amounts of known substances is not included.

This is an area that an affordable spectrometer could target, similar to how the Raspberry Pi targeted programming education. Organisations such as the Royal Society of Chemistry are aiming to better introduce spectroscopy. For example, the RSC offers free "Spectroscopy in a Suitcase" workshops for 16-18 year olds (Royal Society of Chemistry, 2015)

A questionnaire was created to gather further insights on the target market. It covered four main areas: demographics, background and interests, usage and pricing. The full questionnaire is included in appendix A.

Research ethics approval was applied for and granted, and the survey was initially emailed to relevant university societies across the UK. The survey was then posted on scientific interest groups on social media, with subjects including chemistry, physics, astronomy, environmental science and aquariums. 28 responses were gathered in total.

## QUESTION 2.8 QUESTIONNAIRE RESULTS

The target market:

- Is primarily aged **18-35**. This may be biased by the sharing of the survey on social media, where this is the primary age bracket.
- Has a Bachelor's degree or greater. **81% have a Bachelor's degree**, and 48% have at least a Master's degree.
- Is roughly half full-time students, half employed.





Participants' main reason for wanting to use spectrometers is curiosity and experimentation, as had been assumed. Their existing knowledge comes from their education and experience of commercial spectrometers. Most own no spectrometer, but a third of the participants have a commercial instrument. Most interest is in absorption spectroscopy, followed by emission and reflectance, and then fluorescence.

Usage would primarily be in a laboratory setting, so portability is not a major requirement. Manual control is desirable for most participants, with some degree of automation for ease of use. Most participants desired quantitative results, so accurate calibration is important.



Figure 2.8.2: Participants' responses to three different scales.

Participants were shown the specifications for three spectrometers. Spectrometer 1 approximated a low-end Thunder Optics spectrometer, spectrometer 2 was the estimated specification for this project, and spectrometer 3 approximated an Ocean Optics spectrometer. When asked to estimate the price of spectrometer 2, the estimates had a peak around £400, the upper end of the target price range. Coming in below this point will exceed user expectations for value.

Of the three spectrometers shown, half of the participants chose spectrometer 2. This demonstrates a demand for a spectrometer at this price point and capability level. Pixel resolution was a key factor in their choice; users need to choose a spectrometer with a resolution high enough for their usage. Price is less of a factor for those choosing spectrometer 2 than for those who chose the cheapest spectrometer. A built-in user interface is a good differentiating factor compared to the other spectrometers. The wavelength range is not a major factor in most user's decision.

Some extreme users were identified through the survey. A paint company was interested in a portable, self-contained Vis-NIR spectrometer under £400, for use by sales representatives and customer complaint teams. Astronomers desire the ability to fit the spectrometer to a telescope, and require precision in the visible range. Aquarists are potentially interest in taking emission measurements of their lighting, and improving the accuracy of their water testing.

## SECTION 2.9 EXPERT INTERVIEWS

An interview was designed to investigate how experts use spectroscopy, and potentially identify pain points in the existing processes. The questions are available in appendix B. Research ethics approval was applied for and granted by the Brunel Research Ethics Committee

The first expert user interviewed was Dr Terry Ireland, a Brunel Research Fellow in phosphors and nanomaterials. Dr Ireland began with a brief tour of the Brunel Experimental Techniques Centre, showing the variety of spectrometers they use. Notable examples included:

- A small JETI spectroradiometer used for monitoring phosphor performance under different conditions in an environmental chamber
- Spectrometers attached to transmission electron microscopes, so very small areas of the sample can be tested.
- Raman spectrometer with green, red and infrared lasers.

Dr Ireland demonstrated the measurement of a phosphor's emission spectrum using a specialised phosphor spectrometer. This is a typical example of part of his work. Some pain points were identified in this process:

- The spectrometer required a specialised program, from which data was then usually exported to Excel for analysis, despite the analysis capabilities of the program. The program has a software wizard which provides a good step-by-step process, but overlaying multiple spectra is unwieldy.
- Lights had to be turned off in the room for accurate measurement, as the spectrometer was not adequately sealed.

For Dr Ireland's phosphor analysis, a portable spectrometer would not be particularly useful. This is because the purity required for phosphor fabrication requires laboratory conditions, and when in a laboratory he has no need for portability. However, he mentioned that a team had occasionally used portable spectrometers for testing elsewhere.

The second expert user interviewed was Professor Rakesh Kanda, a Brunel Professor in environmental science. He confirmed that environmental scientists do have a use for portable spectrometers. Much of their work is field work, particularly since some tests are only viable for a short time after the sample is taken in the field. For many modern analyses, a UV-sensitive spectrometer is required, but he mentioned that visible-light spectroscopy still has a place in teaching.

Visible light spectroscopy is still used in environmental science for kinetic studies of ongoing reactions, but the usage of spectroscopy is shrinking. Depending on the tests needed, some of Professor Kanda's Ph. D. students still have a use for a Vis spectrometer. For them, price is usually a major factor since they have a limited research budget, and spectrometers can be very expensive. He suggested that home scientists may be interested in drinking water quality parameters.

## SECTION 3 DEFINE

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## SECTION 3.1 USER PERSONAS

Based on the user insights gathered in section 2.7, user personas were created to guide the design process. The idea of the user personas is to represent the variety of users, with some typical and some extreme users. Two examples are included below.

These user personas were used to guide decisions through the design process. Personas enable the designer to "understand, relate to and remember the end user throughout the entire product development process" (Ilama, 2015). They were helpful for keeping the needs of the users in mind.



(Wolpert, 2017)

(Depositphotos, 2015)

### **DAVID**, 33

Works in chemical analysis. Has a BSc and Masters in chemistry. Regularly works with high-end FTIR spectrometers. High level of spectroscopy knowledge.

Wants to: Analyse water quality of his local streams/rivers using standard tests. Wants very quantitative results and full manual control.

Happy to spend a lot of money if he has to. If cheaper options are good enough he will buy them.

### MICHAEL, 20

Doing an engineering degree. Has tried making a DVD-based spectrometer on his phone, but it was too inconsistent. No other spectroscopy experience. Would call himself a "maker".

Wants to: Learn how to use an important analytical instrument. Look at emission/absorption spectra. Interested in qualitative results. On a low budget.

## SECTION 3.2 CONCEPT DEVELOPMENT

To continue the project, the product concept had to be better defined. Ideas so far had ranged from a portable handheld spectrometer for use in the field, to a spectrometer kit for "makers" (Figure 3.2.1). Ideation sketches were combined with discussions with IONICHEM, to refine the concept.



Figure 3.2.1: Initial concept ideation, before Industrial Review Evening.



It was clear that the users came from a variety of backgrounds, and had a variety of needs. A modular design seemed the best choice, as users can select modules that fit their needs. A spectrometer kit may appeal to some users, but many would prefer to concentrate on their investigations rather than making the spectrometer itself the project.



Figure 3.2.3: Investigating component placement and how it affects the spectrometer's form.



## SECTION 3.3 SPECTROMETER TESTING

A basic spectrometer needed to be developed to allow the user interface development to start. The idea of doing this in the Define phase is that it allows time for the design of the supporting parts. The user interface, electronics and external design can all be built around this internal spectrometer.

## **3.3.1 DIFFRACTION GRATINGS**

The basic principles of spectroscopy can be investigated using a diffraction grating made from a DVD. The tracks on the DVD have a fine enough pitch (1350 lines/mm) that the two layers of a DVD-R can be peeled apart and used as a diffraction grating (Public Lab, 2015). Looking at a light source reflected in a segment of DVD shows it split into its spectrum. This can be captured with a mobile phone camera, although there is some difficulty in focusing (Figure 3.3.1).



Figure 3.3.2: Testing 1000 lines/mm diffraction grating using a white LED and a razor blade slit. The diffraction grating is on the nearest mount

This is the basic principle upon which a spectrometer works. There are two main issues with using DVDs as diffraction gratings. One is the curved tracks - tracks nearer to the centre are more curved, and this has to be compensated for in image processing. The second is that production is a difficult manual process.

Fortunately, other low-cost diffraction gratings are available. Diffraction grating plastic film is available in a 35mm slide format, in 600 or 1000 lines/mm. This is a transmission grating - the light is diffracted when passing through, rather than when reflected. A 1000 lines/mm grating was tested by creating frames from foam board (Figure 3.3.2). These frames held the grating and the slit upright and at the level of a mobile phone camera. This allowed the spectrum of a white LED torch to be captured (Figure 3.3.3).



Figure 3.3.3: Spectrum of white LED, taken to test 1000 lines/mm diffraction grating.

## **3.3.2 IMAGE SENSORS**

Tests so far had used a mobile phone camera, which is difficult to align and gave limited control over exposure settings. This led to inconsistent and non-repeatable results. Two different cameras were tested. Both connect to the Raspberry Pi Zero, chosen for its small form factor and large number of connection options.

The first camera was the ZeroCam NoIR. Designed specifically for the Raspberry Pi Zero (The Pi Hut, n.d.), it is extremely small and connects directly to the Pi. It has no IR filter, so it is sensitive past 700 nm, in case the spectrometer's range needs to be extended.

The second camera, the Raspberry PiCamera Module v2 ((Raspberry Pi Foundation, n.d.), is also designed for the Raspberry Pi, but has mounting holes and a more rigid construction. It proved to be more useful due to its rigid mounting holes, and the availability of files for 3D-printing a focusing tool.





Figure 3.3.4: ZeroCam NoIR camera module for Raspberry Pi Zero (The Pi Hut, n.d.).

Figure 3.3.5: Pi NoIR Camera V2 camera module (Raspberry Pi Foundation, n.d.).



### 3.3.3 CARDBOARD PROTOTYPE 1

An enclosed spectrometer prototype was made from cardboard (Figure 4.3.4). The aim of this test was to reduce the light entering the spectrometer from areas other than the slit. This should produce a black background for the spectrum. The box around the spectrometer also aimed to provide some rigidity.



Figure 3.3.7: Spectrum of a fluorescent lamp, captured with cardboard prototype spectrometer.

A graph of the spectrum of the image from this first spectrometer shows wide peaks with little detail (Figure ?). This is because the camera is not focused correctly on the slit. Focusing the lens was difficult because it had to be rotated using needle nosed pliers, and this flexed the cardboard holding it.



### 3.3.4 CARDBOARD PROTOTYPE 2

A second cardboard spectrometer prototype was produced. This test aimed to reduce the size of the box as well as increasing the rigidity. At this stage the length was decreased but the width and height were kept the same, since the diffraction grating was mounted in a 35mm slide holder.

This prototype had two main issues. Despite several attempts to focus it, the image was still blurred. This is due to the relationship between slit size and slit-camera distance. The larger the slit, the larger it will appear in the image. Similarly, the closer the slit is to the camera, the larger it will appear in the image. To compensate for the short slit-camera distance, the slit should have been narrowed.

The large size of the slit in the images causes the spectra to become blurred. A smaller slit image size is required to resolve more detail. This can be accomplished either by moving the slit further from the camera, or by reducing the size of the slit.



### 3.3.4 OPTICAL BENCH

A more rigid and repeatable spectrometer was needed to optimise different parameters of the design. An optical bench was designed to accomplish this (Figure 3.3.9). The diffraction grating is mounted in the centre, and the slit and camera can rotate and move relative to this. An integrated ruler and protractor allowed the distances and angles to be measured. The optical bench was constructed from laser cut MDF and glued together, for increased rigidity compared to the cardboard prototypes.

This level of adjustability allowed a much better result to be reached. Figure 3.3.10 shows the sharp peaks detected by this spectrometer, along with a high contrast between peaks and troughs. The optical bench had mounts for both the ZeroCam and the Pi Camera V2, but the ZeroCam mount was very difficult to hold still when focusing. For repeatability, the Camera Module V2 was used for all further prototypes.



Figure 3.3.10: Spectrum of fluorescent and incandescent lamps captured on optical bench prototype.

By adjusting the angle while watching the live spectrum preview on screen, the spectrum could be centred in the image. This occurred at an angle of roughly 35 degrees. After experimentally determining this, the optimum angle and distances were calculated.

The spectrometer can be simplified to a camera pointing at a slit. The optimal image resolution will be reached when the size of the image of the slit is equal to one pixel on the sensor. The Pi Camera Module V2 has a resolution of 3280x2464 and a sensor size of 3.674x2.760mm, meaning each pixel has a width of 1.12 micrometres. The focal length is 3.04mm.



Figure 3.3.11: Spectrometer design approximated as lens, sensor and slit.

When approximating the spectrometer as shown in figure [?], the slit image width w', lens focal length f, working distance d and slit width w are related by the following equation:

$$\frac{w'}{f} = \frac{w}{d}$$
This equation can be used to find the distance needed for the slit image size to be the same as one pixel. To make the distance shorter a 0.05mm slit is used, the smallest slit feasible to make by hand.

$$d = \frac{wf}{w'} = \frac{0.05 \times 3.04 \times 3280}{3.674} = 135.7mm$$

This measurement is the distance used for later spectrometer prototypes.

The ideal angle between the camera and slit can also be calculated. The diffraction grating equation is:

$$d\sin\theta = n\lambda$$

In this equation, d is the distance between slits on the diffraction grating. is the dispersion angle. n is the order of diffraction (only the first order is used for this spectrometer), and is the wavelength.

With a target range of 400-700nm, the centre wavelength is 550nm. Rearranging the equation allows the angle of diffraction of this centre wavelength to be found.

$$\theta_{550} = \sin^{-1} \left( \frac{550}{1000} \right) = 33.4$$

Note that this is very close to the experimentally determined value of 35 degrees.



— Optical Bench —— USB2000+

Figure 3.3.12: Fluorescent spectrum on Ocean Optics USB2000+ compared to optical bench prototype.

#### **3.3.5 SPECTROMETER COMPARISON**

So far there had been no reference for the performance of the spectrometer. Dr Nadarajah Manivannan provided an Ocean Optics USB2000+XR1 spectrometer for performance comparison. This spectrometer has an optical resolution of 1.7-2.1 nm FWHM, and a range of 200-1025 nm. The 2048 pixels across this range give it a pixel resolution of 0.4nm/px. These specifications mean that it is significantly higher quality than this project is aiming for, which should be useful for comparison.

Figure 3.3.12 shows a fluorescent lamp spectrum captured using both the Ocean Optics spectrometer, and the optical bench prototype. The graph shows a similar level of detail, but the prototype exhibits more noise. Note that the Pi Camera is sensitive to at least 720nm, as evidenced by the small peaks at 650 and 720nm. Figure 3.4.1: Example of image captured by spectrometer.

# SECTION 3.4

An image from the spectrometer is not particularly useful on its own. Two spectrum images may be able to be qualitatively compared, but for quantitative analysis the brightness of each wavelength must be extracted.

#### 3.4.1. SELECTING REGION OF INTEREST

The first step in extracting a spectrum from an image is to crop the image to only the part containing the spectrum. Figure 3.4.1 shows a full image captured by the final spectrometer prototype. Only a small portion of the image is useful data; the rest is black.

It is likely that the useful part of the image could be computed by recognising which areas are always black. However, for this project the image was simply cropped to a region of interest, using the coordinates of its top left and bottom right pixels. This region of interest changes every time the camera moves relative to the spectrometer, so it is important that the camera is rigidly fixed in place.

Early testing used an image editing program to crop the image manually. Between multiple images it proved difficult to keep the cropped area consistent. A code-based solution would be faster and less manual. For this, Python was used for its speed of development and for its support of the Pi Camera Module through the pi camera Python module. In Python, the image is first loaded into a two-dimensional numpy array. This is an array of 8-bit integers (the maximum bit depth of the sensor), and can be easily manipulated to crop the image, as shown below. roi is a tuple with structure ((top\_left\_x, top\_left\_y), (bottom\_right\_x, bottom\_right\_y)).

```
# Crop to region of interest
if roi is not None:
   tl = roi[0]
   br = roi[1]
   y_data = y_data[tl[1]: br[1], tl[0]: br[0]]
```

#### 3.4.2. AVERAGING COLUMNS

As shown in figure 3.4.1, the image has the shorter blue wavelengths on the left and longer red wavelengths on the right. To analyse the spectrum, a single horizontal row of pixels could be taken and their brightnesses used. However, this camera introduces noise to the measurements, particularly when high sensitivities are used.



Figure 3.4.1: Example spectral data.

To combat this, multiple rows of the image were used, and the data in each column was averaged. This averaging should increase the signal to noise ratio.

One disadvantage of this averaging is that it becomes difficult to identify an overexposed image. The value returned by the image sensor for each pixel has a maximum of 255. If too much light was captured by a pixel, the value returned will be 255, and it will be unknown how much more light it should have captured. This is called clipping. The rows of the image are not all at the same brightness. If row 1 is overexposed, by averaging it with rows 0 and 2, its overexposure may be hidden.

## 3.4.3. CONVERTING RGB TO BRIGHTNESS

Once the correct section of the image has been selected, each pixel needs to be converted from an RGB value to a single brightness value. As the camera's image sensor has a Bayer filter in front of it, the image has colour information which is not useful for spectroscopy. For each wavelength a single brightness value is needed.

Several methods were compared for converting RGB values to a single value:

- Basic: brightness = (r + g + b)/3
- Weighted:  $brightness = 0.299 \times r + 0.587 \times g + 0.114 \times b$
- Difference: brightness = |r g| + |g b| + |b r| + r + g + b
- Lightness:  $Y = 0.2126 \times r + 0.7152 \times g + 0.0722 \times b$

$$brightness = 116 \times Y^{1/3} - 16$$

The "basic" method is not a "lossy" conversion - all the information stored in the image transfers to the brightness without being scaled. The rest of the conversions risk throwing away some data.

The "weighted" method is that used by ImageJ (2012), the program used by IONICHEM in the early stages of experimenting with spectroscopy. The source of the weighting values is not known, but different values are used with the same technique for calculating luminance in the d50 sRGB ICC colour calibration profile (Stone, 2013).

"Difference" is the method used by Public Lab's Spectral Workbench online spectroscopy software (Warren, 2012). The final method, "lightness", is the conversion from RGB to the CIE LAB colour space. In the LAB colour space, the L stands for brightness, and A and B encode colour information. In this methods the weighting values are used to approximate human perception of colour.



Figure 3.4.2: Comparison of conversion methods from RGB to brightness, using a fluorescent lamp spectrum.

Figure 3.4.2 shows a comparison of the different conversion methods, after the data was normalised. No single method has a clear advantage over all the others. The "basic" and "weighted" methods greatly exaggerate the brightness of the blue part of the spectrum, compared to the other two methods.

Since there was no clear advantage to any method, the simplest to use was chosen. The pi camera module for Python can automatically provide a YUV image, in which the Y channel represents brightness in the same way as the LAB colour space. This conversion happens on the graphics processing unit of the Raspberry Pi, so it avoids slowing down other computations. This should increase the responsiveness of the spectrometer.

### SECTION 3.5 USER EXPERIENCE IMPROVEMENTS

After using the Ocean Optics spectrometer, observing Dr Ireland's usage, and discussions with Martin from IONICHEM, areas were identified where the user experience needs improvement.

- The process needs to be **streamlined**. The Ocean Optics software makes measurements easy but can be somewhat complex for analysis. With other spectroscopy software, users export into Excel for further analysis. These are extra steps that could be avoided.
- Depending on the user, the process can be **simplified**. A fixed process can be limiting to expert users, but for the average user it may provide the guidance they need for good results.

Both of these could be accomplished by interviewing expert users to define a process for taking (for example) an absorption measurement. The user interface could then be developed to make this process as easy and streamlined as possible. An additional improvement would be to reduce dependency on a connection to a computer. When moving the spectrometer or using in the field, connecting to a laptop can be inconvenient.

### SECTION 3.6 INITIAL SPECIFICATION

#### PERFORMANCE

- Range of 400-700 nm
- Resolution of 5nm FWHM
- Pixel resolution of 1 nm

#### **USER INTERFACE**

- User-friendly interface on spectrometer or connected device
- · Level of control optimised for needs of users
- Should not require wired connection to a computer for operation

#### FORM FACTOR

• Potentially portable or handheld, depending on user needs

#### **MARKET SEGMENT**

- Hobbyist scientists
- Extreme users such as aquarists and plant growers are not an emphasis
- Entry level instrument priced at £200-400

## SECTION 4 DEVELOP



#### **SECTION 4.1 BOX SPECTROMETER** PROTOTYPE

The first "box spectrometer" prototype (Figure 4.1.1) used the dimensions found with the optical bench. The interlocking MDF design made it very rigid, and the camera was held in slots. Loosening the bolts holding it meant it could slide around 10mm in those slots to aid in focusing. Fine adjustment of the camera-slit distance could be achieved without a focusing tool blocking the lens.

This prototype had around 2cm between the diffraction grating and the camera. This meant there was space for a focusing tool in between, but resulted in less dispersion and so a lower pixel resolution on the spectrum. The overall size was also much larger than necessary.



Figure 4.1.2: Box spectrometer fluorescent

This prototype had too short a distance between camera and slit, meaning the image of the slit covered multiple pixels. The effect of that is that the peaks of a fluorescent lamp spectrum are rounded, as shown in figure 4.1.2.

Another improvement this iteration brought was the ability to connect fibre optic cables. By changing the two front pieces which connect outside the slit, an Ocean Optics fibre optic cable can be attached, or a low-cost 1mm acrylic fibre optic. Connecting fibre optics to the spectrometer allowed it to join to other attachments.



Figure 4.1.3: Laser pointer holder and cuvette holder.

A cuvette holder and laser pointer holder were also laser cut from MDF. The cuvette holder allowed the first absorption measurements to be taken. Figure [?] shows the absorbance for each wavelength. Note that there is negative absorbance - less light reached the spectrometer through the distilled water than through the ink sample used. This is unusual, and potentially due to the ink samples scattering light. However, the region between 490 and 570nm is still usable.



Wavelength / nm



## BOX SPECTROMETER PROTOTYPE 2

This prototype aimed to address the problems with the previous spectrometer, particularly the size and slit-camera distance. This design was based around a slit-camera distance of 135mm, to match the calculated optimal value for a 0.05mm slit. The diffraction grating was moved as close to the camera as possible to increase dispersion and spectral resolution.

Figure 4.2.1 shows the size reduction with the newer prototype. The width and height have been reduced from 50mm to 38mm. Despite this size reduction, the optical path is much longer, increasing the optical resolution.

An improved fibre optic connector was created for this prototype. The 1mm fibre optics had been useful for connecting parts, but the actual connection had been inconsistent. To remedy this, a TOSLINK connector was designed in Rhino. This connector (Figure 4.2.2) improved the rigidity and repeatability of the connection to the fibre optic cable.



Figure 4.2.2: 3D-printed fibre optic connector.

#### **SECTION 4.3 MODULAR DESIGN**

A modular design reduces the range of products IONICHEM need to make to cover all needs. Instead of manufacturing a variety of specialised spectrometers, one spectrometer can be produced with a variety of modules. These modules could include different types of light source for targeting different wavelength ranges. Another option could be a module with lasers or a fluorescent lamp for wavelength calibration.



Figure 4.3.1: Modular design sketches.



Figure 4.3.2: Sketches illustrating degrees of modularity.

#### 4.3.1. DEGREE OF MODULARITY

A relevant concept is the degree of modularity. A product can be completely non-modular, and be a single unit. Alternatively it could be completely separated into its component parts, or somewhere in between. To apply this to a spectrometer, it could be a single unit optimised for absorption measurements through a cuvette. The light source and cuvette holder would both be built into the spectrometer.

A fully modular spectrometer could have its light source, cuvette holder and spectrometer as separate modules. Additional modules could include screens and power supply or battery options. This type of modular system can be very complex to design, but can allow the user to configure the system to exactly fit their needs. This is too complex for the scope of this project, as connectors can be difficult to design and troubleshoot.

A good middle ground is a semi-modular design. The spectrometer unit can be separated from the sample unit, but the sample unit contains both the cuvette holder and the light source. This demonstrates the potential of a modular design, while only introducing the complexity of a single modular connector.

#### 4.3.2. MODULE CONNECTOR

The modular connector designed for this spectrometer had several requirements:

- Optical connector to transfer light between sample and spectrometer
- Electrical contacts to power lamp
- Consider support for future modules
- Keyed to prevent incorrect orientation

The optical connector selected was the TOSLINK standard. This is due to the relative abundance of TOSLINK cables due to their use in optical audio. These cables usually contain a 1mm acrylic fibre optic, which is large enough to transmit a significant amount of light.

The halogen lamp used in the spectrometer requires only two contacts: +12V and ground. Future "smart" modules may require a digital communication protocol, for example to control motors or to sequence different light sources. For these, the connector would need to be designed with additional contacts. These could include a +3.3V and +5V for microcontrollers, and SDA and SCL pins for an I2C bus. An I2C bus allows communication of up to 128 different devices on the same two pins.



Figure 4.3.3: Connector mechanism ideation.

The overall shape of the connector needs to be keyed so that it can only be connected the right way. This reduces the likelihood of damage to the optical and electronic connectors (in particular, preventing shorting the electrical contacts). The shape of the connector body can also be used to guide the TOSLINK connector into place, by bevelling both sides. This ensures that the two parts correctly locate against each other, ensuring consistent positioning of the fibre optic.



#### SECTION 4.4 USER INTERFACE

User interfaces of existing spectrometers are very varied. All lowcost spectrometers discovered in the research for this project require connection to a computer, so a more portable user interface is a major differentiating factor. With the ever-rising popularity of phones, tablets and devices like Chromebooks, Windows-specific programs are a limitation. This is not usually a problem in a professional setting, but in a home lab where the user may prefer other operating systems it is inconvenient.

Two remaining options are a built-in user interface (on a touch screen or buttons) or an app-controlled spectrometer. A built-in interface increases the cost of each spectrometer, but offers a consistent and always-available experience. An app for phones or computers (hereafter grouped together as "smart devices") has the advantage of being able to be updated in future, unlike a physical interface. However, the major disadvantage is that updates are required to keep the app working as devices update. For a small company like IONICHEM, a lower-maintenance solution than an app is a website. Modern browsers still support websites dating back to the creation of the World Wide Web in 1990. In contrast, apps from as little as two years ago are not supported on modern devices. Since the spectrometer is based around a Raspberry Pi, which is a small computer, the spectrometer itself can host a website that the user can use with any smart device.

To implement this, a "web stack" needs to be used, so that the "backend" on the spectrometer can communicate with the "frontend" on the connected device. For this, the Python module flask was used, due to the author's familiarity with Python. Flask is designed for creating webapps, and only a basic one is needed for this use.

In a basic website, the content is loaded once when the page first loads, and no further change happens. Of course, for a spectrometer with a constantly changing spectrum, this is not very useful. The page would have to be constantly refreshed to update the graph. The socketio module was used to allow the Javascript code running on the connected device to communicate with the spectrometer's Python code.

As an example, here is the Python code to turn on the lamp when a device connects:

```
@socketio.on("connect", namespace="/spectrometer")
def signal ClientConnect():
    """
    Signal to the power management PIC that a client
is now connected
    """
    print("Client Connect")
    gpio.output(extra1, True)
```

The signalClientConnect() function is run when the "connect" event occurs, which is when a device loads the spectrometer website. The function simply logs the message "Client Connect" and turns on one pin of the Raspberry Pi. Other functions deal with requesting an updated spectrum, and sending the updates.

#### SECTION 4.5

## SMART DEVICE CONNECTION

To host a website, the spectrometer needs to be connected to the same network as the smart device. There are three ways to do this:

- Separate WiFi network, to which both spectrometer and smart device are connected.
- WiFi network **hosted by smart device**, to which the spectrometer connects.
- WiFi network **hosted by the spectrometer**, to which the smart device connects.

The problem with the first two options is that the spectrometer must know the name and password of the network before it is able to connect. With no user interface on the spectrometer unit, this would be difficult. The third option means that the spectrometer will never be able to have an internet connection, as only one WiFi connection can be made per device. This means updates become difficult (requiring connecting a USB drive or similar).

Hosting a WiFi network on a Raspberry Pi has two parts. The first is creation of the network. The program hostapd makes hosting a WiFi network simple, and a network was set up with the name "Spectrometer" and password "IONICHEM".

The second part is assigning IP addresses to connected devices. The DHCP protocol is in charge of this - a Raspberry Pi can host a DHCP server. Two different DHCP servers were tested (isc-dhcp-server and dnsmasq), but this step was unsuccessful. Without an IP address the smart device cannot connect to the website hosted by the Pi.

As an alternative, the user is directed to create a WiFi hotspot on their smart device with a known username and password. The Raspberry Pi will automatically connect to this network. This would not be acceptable for a commercial product, but for a prototype it is sufficient.



Figure 4.6.1: Spectrum of clear and blue halogen lamps.

### SECTION 4.6 OPTICAL DESIGN

There are few small halogen lamps available. A standard W5W halogen bulb used for small lights in vehicles was the most appropriate bulb found. This runs at 12V and 5W, and is a type of incandescent bulb. This means it puts out a limited amount of blue light. Bulbs are available which attempt to produce a whiter light, by coating the bulb in a blue filter. This attenuates the green-red light, and lets the small amount of blue light output by the bulb pass (Figure 4.6.1). This would be worth investigating in future.

Next, as much light from the lamp needs to enter the fibre optic as possible. A test was created using a mirrored plastic film surrounding the lamp to make a reflector. The reflector was focused on the end of a fibre optic based on simple geometry - the angle of incidence equals the angle of reflection. The light output at the other end of the fibre was measured using a light-dependent resistor connected to an Arduino. The resistance of the LDR is roughly linearly correlated with light hitting it.



The reflector tested did not succeed in directing significantly more light into the fibre optic. As an alternative approach, several lenses were tested to focus the lamp's light into the fibre. The most successful of the lenses had a diameter of 5.5mm, a focal length of 4.5mm, and was placed around 4.5mm from the fibre optic. This small size was ideal, as it helps to minimise the spectrometer's size. The lens increased the amount of light entering the fibre optic by 37%.

To further improve the optical coupling from lamp to fibre, the ends needed to be polished. After cutting with a knife or scissors, the ends are rough and translucent. A small brass block was created on the lathe to hold fibre optics at 90 degrees to the polishing surface. The fibres could then be ground flat on a 1000 and 4000 grit stone, before polishing with abrasive compound on a leather strop. A polished fibre optic end is more transparent than a rough one, so more light will enter or leave the fibre.

The second box spectrometer prototype had an issue when a very bright light source was used. The light could reflect off the side of the box, creating false readings. To reduce the amount of light, baffles were added to the sides of the box. Figure 4.6.3 shows the planned structure of the baffles.



Figure 4.6.3: Internal baffle layout. Only three pairs were added to the final design.

It was unlikely that the distances when manufactured would be perfect. For that reason some adjustment is needed, to correctly focus the lamp onto the fibre optic. The 3D-printed pieces were designed to mount on a miniature optical rail, with slots to allow them to be adjusted back and forth. Bolts on the underside lock them into place. This proved to be difficult to use. A better option would be to have micrometric screws in the mounts, to provide fine and repeatable adjustment.



Figure 4.6.4: Optical rail used in final spectrometer. Lamp holder and lens holder are moveable, cuvette holder is fixed.



Figure 4.7.1: PIC16F1827 power management circuit.

#### SECTION 4.7 POWER MANAGEMENT

The Raspberry Pi in the spectrometer needs to be powered down gracefully or it risks data corruption. As it is essentially a small computer, the operating system needs to be triggered to shut down (similar to clicking "shut down" on a desktop PC rather than pulling the plug). Shutting down takes around half a minute. Once shut down, the power can be disconnected.

This power switching can be done using a simple MOSFET circuit (Othermod, 2016). However, the downside of this circuit is that there is little feedback to the user while it is working. There is no indication that the Pi is starting until the Pi can switch on an LED, which takes around a minute from initial power-on. Similarly, it is difficult to tell when the Pi has fully powered off.

Instead, a microcontroller can be used to control power to the Pi using a MOSFET, as well as a feedback LED. Because the microcontroller is very low power, it can be left running even when the Pi is switched off. There is little to no risk of data corruption when the microcontroller's power is disconnected abruptly. The main advantage of using a microcontroller to control the power and the feedback LED is that it is independent of the power state of the Pi. Feedback can be given to show the user the Pi is starting, long before the Pi is ready to do so.

### SECTION 4.8 FINAL SPECIFICATION

A product design specification was created from the research and development of the project. The final specification is available in **APPENDIX** ?.

## SECTION 5 DELIVER



Figure 5.1.1: Exploded view.

#### SECTION 5.1 PHYSICAL DESIGN

The insides of the spectrometer were modelled in Rhino, and around this a rough version of the external design was created. This was then re-created as a parametric model in Creo, to allow CNC milling of the final prototype casing.

The case is designed to match the name: IONICHEM Wave. It uses a calm blue-and-white theme and wave motif on each section. The top surface curves down to make a 45 degree angle with the ground, against which a phone or tablet can be rested.







Figure 5.1.3: Milling device holder slots.





#### SECTION 5.2 USER INTERFACE

An interview was conducted with Martin Teasdale from IONICHEM to determine the steps needed to take an absorption measurement. These steps were recorded and translated into a set of screens that would be required.

These screens were arranged into a wireframe, with arrows to show where each button would take the user. The wireframe was converted to a PDF with clickable links between the different screens. This PDF was tested with Mr Teasdale and iterated upon. The final wireframe for the user interface is shown to the left.

The working prototype of the user interface is loaded on the spectrometer, and has a simple emission graph, which is updated every half a second. The shutter speed and sensitivity can be adjusted using text boxes at the bottom of the screen.



# SECTION 5.3

A user guide was created to show how the prototype can be operated. It covers setup, basic usage and correct shutdown of the unit. A final product would need a much more comprehensive user guide, including troubleshooting steps for common issues.



Figure 5.4.1: Final absorbance spectrum

#### SECTION 5.4 FINAL TESTING

The final prototype was tested by taking absorbance measurements of a set of blue ink samples provided by IONICHEM, and comparing a calibration curve constructed from these samples with that of an Ocean Optics USB2000+, as well as IONICHEM's WPA commercial spectrometer. Figure 5.4.2 shows that the sensitivity of the IONICHEM Wave is much lower than the other two spectrometers, but the response is more linear than that obtained on the Ocean Optics spectrometer. Linearity means the calibration curve is useful for calculating the concentration of an unknown sample.



Figure 5.4.2: Comparing calibration curves





# SECTION 6

The final spectrometer design was compared with the specification. Some features, such as the full user interface, were designed but not implemented in the prototype. For example, "the product must generate a graph of absorption against wavelength." This was not implemented in the software prototype, but is included in the user interface wireframes. The user interface which was wireframed and prototyped can do the tasks specified. The working prototype can only do a simple emission measurement, which is adequate as a proof-of-concept.

The spectrometer meets the target for a spectral range of 400-700nm, and can even be extended to 800nm. The pixel resolution also exceeds the specified 1nm. However, the prototype's sample rate and latency are not not as fast as specified. Both are around half of the desired level - 2Hz sample rate instead of 4Hz, and 1 second latency instead of 0.5 seconds. This is due to the image processing required, which is not very fast on the Raspberry Pi Zero. It is possible that it could be optimised by writing the image processing in a language other than Python, or by using a more powerful processor inside.

The target price was set at £200-400, with users expecting to pay £400 for a similar spectrometer. The parts cost for the final prototype comes to £50 for the internal parts. The cost of the casing has not been calculated as it would not accurately reflect the injection moulded casing used on a final product. Once optimised bought in bulk, the parts cost should be halved, for an estimated total materials cost of £30. With an instrument such as this which requires calibration, labour would be significant and the manufacturing cost per unit would be at least £60, including parts. This is likely to be too high to meet the low end of the price point, as it is recommended that the manufacturing cost is less than 30% of the sales price to account for transport, administration and

packaging overheads, as well as profit. Due to this, the final sales price is estimated at £300.

The final prototype has a high quality finish. With more development of the user interface running on the prototype, it could be used as a proof-of-concept to interested parties.

#### 6.1 FEEDBACK FROM IONICHEM

The prototype was demonstrated to Martin from IONICHEM over a video call. Overall, he was very happy with the prototype, and mentioned that he had potential business partners interested in seeing a working prototype, once the user interface is more developed.

As a key differentiating factor of the product, Martin noted that the user interface requires significant further development. In the short term, the basic functionality working is good enough. The usability of the software is key and the PDF prototype is a good start, but as we develop it the feature could become the main unique selling point of the spectrometer.

Future development work Martin suggested included different modules with a variety of light sources and sample holders. Using a linear diode array instead of an image sensor would greatly improve the sensitivity and response time of the spectrometer, and would greatly reduce the complexity of the image processing. This might be something to investigate as an option to differentiate the product line, between "professional" and "hobbyist" products.

#### 6.2. FUTURE DEVELOPMENT

A useful future development would be a better light source. Directing more light into the fibre optic would allow a faster response of the spectrometer, which is key to the user's opinion of how well it works.

The user interface prototype needs significant improvement, particularly the setup process. If the spectrometer could create its own WiFi network, the whole process would be much simpler. An update strategy needs to be considered. While a website requires less updates, some may still be needed. The software could be updated using a USB drive, or by connecting the spectrometer to a computer.

The connector needs to be made more consistent. There is some play in the placement, which can allow readings to be slightly altered when moved. Improving the connector would also give the opportunity to add other electrical connectors to support future peripherals.

Overall, this has been a worthwhile project and demonstrates the quality even a low-cost spectrometer can achieve. The initial goal of investigating whether a modern webcam can reach "good enough" results has been achieved, and it was a success. The project is planned to continue with IONICHEM, until a fully working prototype is ready to demonstrate to their business partners.


The following pages contain the user questionnaire questions.

# APPENDIX B

The following pages contain the interview used for expert users.

### PARTICIPANT INFORMATION SHEET

As someone who works with spectrometers, you are invited to take part in this research interview. Before you decide, it is important to understand why the research is being done and what it will involve. Please take time to read the following information carefully and discuss it with others if you wish, and then decide whether or not you wish to take part. Ask me if there is anything that is not clear or if you would like more information. You can cancel your participation and withdraw your information at any point.

I am George Bryant, a final-year Product Design Engineering student at Brunel University, gathering insights for my final project. This project is focused on making optical spectrometry more accessible to amateurs and hobbyists. The responses gathered through the questionnaire will be used to gain an understanding of the market, which will guide the design process.

Data from the interview will be protected under the Data Protection Act. All data gathered will be made anonymous, and will be retained until the close of the project, upon which it will be reviewed and deleted.

If you need any further information about the interview or project, please email George Bryant at 1418415@brunel.ac.uk

### **CONSENT FORM**

By taking part in this interview, I consent to use of the information I give in the researcher's project. I understand that all data will be kept confidental, and my personal information will not be stored. I am free to withdraw at any point, including after the interview, without giving a reason.

I consent to publication of study results as long as the information is anonymous, so that not identification of participants can be made. The study has received approval from the Brunel Research Ethics Committee.

I have read and understand the explanations and I voluntarily consent to participate in this study.

Name: \_\_\_\_\_\_

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If you need any further information about the interview or project, please email George Bryant at 1418415@brunel.ac.uk

### **INTERVIEW QUESTIONS**

1. Do you work with visible light spectrometers?

- If no skip to question 10.

2. What fields do you work in?

3. What do you use visible/near-IR spectroscopy for in your work?

4. In what situation would you use Vis/NIR spectroscopy instead of other analytical methods?

5. Is there a particular area where it's most useful?

6. What Vis/NIR spectrometers do you currently use?

7. How frequently did you use them in the last month?

8. Could you walk me through the steps you'd take to analyse a sample using [one of the spectrometers they use]? Where possible this will be done at the actual spectrometer.

9. Does any part of that process get tedious or repetitive or annoy you?

- Is any of it difficult?

- Is there anywhere you sometimes press the wrong thing?

10. Do you have any interest in spectroscopy outside of work?

11. If you were looking for a spectrometer for use outside of work,

what would your requirements roughly be?

- Could you put those in a rough order of priority?

- If needed, prompt: "Price", "range", "resolution", "any particular software features?", "anything it would need to connect to?"

12. Would a spectrometer being portable or handheld add anything for your use?

13. Would spectrometer size matter to you for home use?

14. Do you have any other comments on spectrometers, either at home or at work?

15. What do you think a home user might potentially use a spectrometer for?

16. Do you know anyone else who might have interesting opinions or information for this project?

### APPENDIX B FINAL SPECIFICATION

#### 1 Features

1.1 The product must generate a graph of light intensity against wavelength for a light input.

1.2 The product must also generate a graph of absorption against wavelength using a light input through a cuvette holder holding a sample.

1.3 The spectrometer unit will be a modular platform. Three modules are in the scope of this project: Processing, cuvette holder and lamp modules.

1.4 A user interface will be displayed on a connected "smart device" (phone/tablet/laptop/etc). Optionally, there will be a basic user interface on the spectrometer for measurements without a connected smart device.

1.5 Automatic calculation of absorption values across wavelength range.

1.6 Based on a Raspberry Pi, with wireless connection to the user's smart device.

1.7 Database of specific chemical tests to have spectrometer automatically select correct wavelength range, and the ability to define custom tests.

1.8 Cuvette holder for standard 12mm x 12mm cuvettes

1.9 Lamp for absorption spectroscopy of liquid samples

1.10 Attachable fibre optic cables for connection to external optics, instead of cuvette holder

2 Performance

2.1 Spectral range of 400-700 nm, and spectral resolution of 5nm FWHM.

2.2 Pixel resolution of 1 nm.

2.3 Sample rate greater than 4 Hz, exposure-to-screen latency less than 0.5 seconds, when not limited by exposure time.

3 Target Market

3.1 Hobbyist scientists, primarily chemistry and physics enthusiasts. Survey responses were primarily chemistry and physics enthusiasts.

3.2 Primarily aged 18-35, with a Bachelor's degree or greater.

3.3 Roughly half full-time students, half employed.

3.4 Secondary markets include aquarists and paint/print colour matching.

4 Price

4.1 The target price set by IONICHEM is £200-400. The user expectations in a survey were found to be £400, matching the upper target price.

5 Business Model

5.1 This is a collaborative project with IONICHEM; the company may develop the product further. The following are potential parts of the business model.

5.2 IONICHEM will sell to hobbyist scientists and small businesses, either distributing directly or in partnership with other companies.

5.3 IONICHEM may have support contracts with customers, including bespoke customisation of user interface or spectrometer features, or additional modules.

5.4 Potential future developments include a higher-end instrument aimed at professionals, with a similar user interface and higher quality components for more precise results.

5.5 The market position will be between cheap low-resolution spectrometers, and higher-end offerings by existing spectrometer manufacturers such as Ocean Optics.

6 Product Lifespan

6.1 The product should last at least 5 years of use, with an average power-on time of 2 hours per week for hobbyists, or 10 hours per week for business users.

6.2 The bulb lifetime will be lower (~450 hours) and so must be easily accessible.

7 Aesthetics

7.1 Styling should be appropriate for use in a laboratory, to fit with other laboratory equipment.

8 Ergonomics

8.1 All controls of the spectrometer must be reachable from the spectrometer's resting position on a table, from a seated or standing position. This will be verified with Jack Virtual Human.

8.2 Must be able to be carried to difficult-to-access remote locations. Maximum size 20x10x10 cm. Maximum weight 500g – a comparable Ocean Optics Flame-Chem weighs 445 g.

9 Interface Requirements

9.1 A detailed user interface must be available as a website hosted on the spectrometer. The following are tasks the UI should enable the user to do:

9.2 View graph of intensity of wavelengths, or of absorbance, across measured spectrum.

9.3 Select test from database of common tests, and add to test database. The test will define the peak wavelength being measured.

9.4 Select number of measurements to average for noise reduction.

9.5 Adjust exposure time / sensitivity, or enable automatic control.

10 Product Environment

10.1 The primary product environment is a home or small business laboratory.

10.2 Liquid samples are commonly used, so the product must be water resistant.

10.3 Should be at least IP53 rated: 5=Dust ingress minimised, 3=Safe with spraying water.

11 Maintenance and End-of-Life

11.1 Spectrometer and accessories should be connectable using commonly-available TOSLINK fibre optic cables.

11.2 The bulb should be readily available and easy to replace: T10 W5W halogen bulb.

11.3 Modular parts must be able to be separated without tools. All electronics should be accessible for repair by technicians or advanced users, using only (Philips/hex/Torx) screws.

11.4 The main parts (Processing board, power supply circuitry, image sensor, grating) should be able to be removed for maintenance or at end of life, for reuse, repurposing or recycling for easier compliance with the WEEE directive.

12 Health & Safety

12.1 Electrical safety: Ensure any mains voltages are separated

from the "wet area". The spectrometer unit itself will be doubleinsulated with full plastic enclosure and so will not require grounding.

12.2 Fire safety: Included lamp must be adequately cooled, and should remain below 90°C at all times during operation. If temperature increases beyond this airflow solutions should be added to keep it below this threshold. No flammable materials may be located within 3cm of the bulb.

12.3 Laser safety: Ensure any lasers are enclosed and cannot be directed anywhere other than into the spectrometer. Lasers should be class 1 or class 2, with power below 1mW. Lasers should be used for calibration only.

13 Materials

13.1 The main body should be made from non-porous plastic such as ABS for electrical insulation and to prevent water ingress.

14 Manufacturing Process

14.1 The casing of the product will be injection-moulded or made using pre-made enclosures.

14.2 The product will be assembled at small scales by hand, as it is low-volume.

15 Quality Standards Testing

15.1 The range and sensitivity of the spectrometer will be calibrated using a comparison with an Ocean Optics USB2000+ spectrometer.

15.2 The range will be calibrated using a light source (Fluorescent lamp) producing at least 6 spectral lines within the range of the spectrometer, as recommended for calibration of the USB2000+. The locations of each peak in pixels will be measured and a third-order polynomial best fit used to find the relationship between pixels and wavelength.

15.3 The sensitivity of the spectrometer will be measured by calculating its signal-noise ratio.

15.4 The two spectrometers will also be compared by using the absorbance of a set of reference samples provided by IONICHEM to generate a calibration curve for each. The calculated concentration (for an unknown sample) from this product should be within 20% of that of the USB2000+.

16 Power Supply

16.1 The unit will be powered by an external mains-isolated 5V or

12V power supply.

16.2 If 5V, external power supply will be a typical micro-USB or USB-C phone charger. A boost converter will be used to step up the voltage to 12V to supply the spectrometer lamp.

16.3 If 12V, external power supply will be a laptop-style power cord with a barrel jack connector. A buck converter will be used to step down the voltage to 5V for the digital logic.

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## **BUSINESS PLAN**

### SECTION 1 THE BIG IDEA

### 1.1. THE PROBLEM

Optical spectroscopy is used in a laboratory setting for finding the concentration of known substances in a sample. It is so widespread that most chemistry laboratories will have at least one spectrometer, if not several of different kinds. However, spectrometers tend to be expensive, and hobbyists who want to try spectroscopy have little choice but to save up. In recent years some low-cost, semi-DIY options have entered the market, but they are not high enough quality for much more than satisfying curiosity. The chemical analysis company IONICHEM provided the brief for this project.

### **1.2. THE PRODUCT**

The IONICHEM Wave is a spectrometer aimed at hobbyist scientists. It supports the most common spectroscopy methods (absorption and emission), and costs only £300. The spectrometer connects to a smart device (phone, tablet or PC) to display an intuitive user interface. No software installation and little setup is required.

### **1.3. INNOVATION TYPE**

The innovation type of this project is primarily product innovation. The aim was to bring recent advances in low-cost image sensors to a spectrometer, and bring the functionality of higher-end devices to a price range affordable to hobbyists.

The innovation of this product is incremental. Spectrometers already exist with better capabilities or at cheaper price points, so this is largely an exercise in creating a different balance of those two factors.

### **1.4. SWOT ANALYSIS**

Strengths:

• Streamlined user interface for measuring samples.

• Connects to a phone or tablet to show user interface, so a PC is not required.

• Brings functionality to the market usually only available at a higher price point.

Weaknesses:

• Many established companies with a lot of brand trust are already on the market.

• There are few attachments compatible with the spectrometer.

• Spectrometer is less sensitive than professional options.

**Opportunities:** 

• Nothing on the market that brings a good user interface to a non-professional spectrometer.

• Low cost makes it accessible for students, teachers, hobbyists. Threats:

• Existing companies may be able to rapidly outcompete the product if they decide to enter this part of the market.

• Very niche market, where most advertising is by word-of-mouth or relationships with suppliers.

• No market recognition except from IONICHEM's few existing contacts.

### **1.5. CURRENT ALTERNATIVES**

There are four main sets of current options for a hobbyist scientist:

• Entry-level spectrometers from established companies, like the Ocean Optics USB2000+. These start at around £750, even used.

• Cheap "curiosity" spectrometers like the Thunder Optics Mini USB spectrometer. Without the ability to attach to anything or developed software, these are not much more than toys.

• Kits or DIY options such as the Public Lab Desktop Spectrometry kit. These can provide good results, but only if the user creates a good enclosure for them.

• Single-purpose testers such as the Hanna lodine Portable Photometer. These will provide high quality results when testing for a specific chemical. Buying multiple for different tests becomes

#### expensive very quickly.

#### 1.5.1. PERCEPTUAL MAPPING



• This highlights the gap in the market for a versatile and cheap spectrometer

• The reason that hasn't been done is that "versatile" tends to equal expensive. Consumers will expect products put out by an established company to be very high quality.

• Modern camera technology may mean that such a setup is viable, particularly for non-business users .

### **1.6. UNIQUE SELLING POINT**

· More versatile than existing options in this price range

• A full-featured spectrometer at a price for which you would normally be able to buy a device which tests for a single substance.

• Has an intuitive user interface that doesn't require connecting to a computer.

### **1.7. EXAMPLE USER PERSONA**

Clive is 30 and has a standard office job. At home he has several aquariums, and he would like to take a more scientific approach to managing them. He doesn't have any previous spectroscopy experience, but he's interested in learning. Clive has trouble with chemical test kits because he's slightly colourblind, so he wants to verify their accuracy. Used to test kits being expensive, so happy to pay a high price.

### SECTION 2 BUSINESS MODEL

### 2.1. MARKET SEGMENTATION

ite. Video demonstrations of product usage on website and YouTube. Indirect: People talking to existing customers on social media.

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• Very niche market

• Hobbyist scientists are difficult to quantify, as they are usually not very vocal.

- Core market is chemists and environmental scientists
  - Primarily 18-35 years old
- Secondary markets
  - •Aquarists
  - Astronomers
- Tertiary markets
  - Small businesses such as paint mixing companies
  - Schools (possible future expansion of markets)
    - May use profits from other markets to sell to education at
- a loss
- Individual consumers
- Mostly UK-based, since distribution and support is difficult across borders

### 2.2. VALUE PROPOSITION

#### USABILITY

Proposed user interface makes it easier to measure your samples.

#### VERSATILITY

Can do much more than the single-purpose photometers in a

similar price range.

#### CONVENIENCE

Not needing to connect to a full computer makes it much easier to get started.

#### PRICE

For most users, the value they get out of it will be the same as better spectrometers, but at a lower price.

### 2.3. CHANNEL PHASES

#### 2.3.1. AWARENESS

Direct: Contact partners to arrange distribution deals. Potential crowdfunding. Indirect: Word of mouth online and in person.

The right established distributor will likely be able to raise awareness more effectively than IONICHEM alone. Crowdfunding would both generate awareness and allow IONICHEM to gauge interest, even before the final product is released.

#### 2.3.2. EVALUATION

Direct: Information on website. Video demonstrations of product usage on website and YouTube. Indirect: People talking to existing customers on social media.

Ocean Optics offer particularly in-depth spectroscopy information on their website, which is very helpful. This could be emulated and coupled with a video social media presence, so that potential users can see how easy the product is to use.

#### 2.3.3. PURCHASE

Direct: Direct sales on website or by phone. Possibly in crowdfunding campaign. Indirect: Through deals with distributor/partner

#### 2.3.4. DELIVERY

Direct: Advice on website on how to use the product for the best results

#### 2.3.5. AFTER SALES

Direct: Email customer support, and repair service. Indirect: Partners may offer paid support and servicing.

### 2.4. CUSTOMER RELATIONSHIPS

#### PERSONAL ASSISTANCE

Support available by email for customers needing help.

#### **DEDICATED PERSONAL ASSISTANCE**

Direct in-person support and servicing. May be a paid service.

#### COMMUNITIES

The IONICHEM website hosts a forum for existing and potential product users.

### 2.5. REVENUE STREAMS

#### **ASSET SALE**

The user buys the spectrometer for £300.

#### **SUBSCRIPTION FEES**

The user can pay for on-demand support. The cost would depend on the type of support needed and the type of user. For example, a home user is likely to need support less often than a business customer with multiple users.

### 2.6. KEY ACTIVITIES

#### **FUNDING FROM PARTNERS**

Partners need to be approached for funding and support, in exchange for a percentage of the profit.

#### **PRODUCTION**

The spectrometer needs to be manufactured

#### **PLATFORM**

The website must be created, as well as the information videos hosted on it.

#### PROMOTION

Ideally most promotion would be done by distributors, but initially some word-of-mouth interest will need to be generated by sharing information about the product on social media.

### 2.7. KEY RESOURCES

#### PHYSICAL

Facilities to manufacture the product, warehouse space to store it for distribution, office space for administration.

#### INTELLECTUAL

IONICHEM is a registered company, but the IONICHEM Wave brand should be trademarked.

#### HUMAN

Industrial designer and design engineer for the physical design of the product. UX designer to design the user interface. Web developer to develop the user interface. Electronics engineer to design the electronics. Optical engineer to optimise the spectrometer.

#### **FINANCIAL**

Loans/investments from distributors. Possible financial support from crowdfunding.

### 2.8. KEY PARTNERS

#### DISTRIBUTOR

As a small company in a niche market, it will be difficult to gather interest. IONICHEM's current preference is to create an agreement with a distributor to increase the number of people viewing the product. This should also reduce the risk of failure due to few potential customers seeing the product.

### 2.9. COST STRUCTURE

The cost of the prototype spectrometer was around £60. Due to economies of scale, in large volume component cost will be significantly reduced, but labour cost needs to be included. Overall manufacturing cost is likely to remain close to £60, since this type of product requires manual calibration.

The remaining £240 from the sale of each product needs to cover marketing, development costs, support and administration personnel, transport and other overheads. The profit remaining depends on the percentage that the distributor demands.

### SECTION 3 RISK MANAGEMENT

Area	Potential risk	Impact	Probability	Priority	Action
Distribution/ funding	Unable to secure partners	High	Medium	High	Consult with multiple distributors to ensure a deal is reached before much further investment.
Intellectual property	Established company creates similar product	High	Low	Medium	Ensure that adequate IP protection is taken out. The right patents should limit the likelihood.
Manufacture	Delays in production	Medium	Medium	Medium	Re-evaluate the production process and consider alternatives to problem steps.
Manufacture	Poor manufacturing quality	High	Medium	High	Create quality assurance procedure to catch low production quality as soon as possible.
Technical	User interface has poor device compatibility	Medium	Low	Low	Hire a consultant web developer to ensure compatibility with modern devices.
Marketing	Not enough users are interested to make a profit	High	Low	Low	Apply for more investment and adapt marketing campaign. Consider pivoting the product to tertiary markets.