

Article

Using Multispectral Imaging to Reveal the Relationship between UV Absorbance and Sulphur Dioxide Concentration

Keru Lu ¹, Zhilin Li ^{1,2} and Man Sing Wong ^{1,*} 

¹ Department of Land Surveying and Geo-Informatics, The Hong Kong Polytechnic University, 181 Chatham Road South, Kowloon, Hong Kong

² Faculty of Geosciences and Environment Engineering, Southwest Jiaotong University, Chengdu 611756, China

* Correspondence: lswong@polyu.edu.hk; Tel.: +852-3400-8959

Abstract: The sulphur dioxide (SO₂) concentration can be monitored via its absorbance in the ultraviolet (UV) region. To address the absence of a systematic study on the UV absorbance of varying SO₂ concentrations, a multispectral imaging method was implemented in the present study. SO₂ concentrations and various environmental conditions were controlled by a purpose-built environmental control system with a light path of 4.2 m. Five narrow-band-pass filters in front of a UV camera were used to implement multispectral imaging. Regression models of the relationship between UV absorbance and SO₂ concentration at each wavelength are presented. Their residuals were kept relatively small by adopting Jenks natural breaks analysis, with a maximum standard deviation of 0.086. Temperature and SO₂ concentrations were significantly associated with UV absorbance. Furthermore, smoothed look-up tables were developed to explicitly elucidate the correlation between UV absorbance and SO₂. These have been represented as heat maps, showcasing an example of library construction using a combination of abundant research data.

Keywords: sulphur dioxide; multispectral imaging; UV absorbance



Citation: Lu, K.; Li, Z.; Wong, M.S. Using Multispectral Imaging to Reveal the Relationship between UV Absorbance and Sulphur Dioxide Concentration. *Sustainability* **2023**, *15*, 138. <https://doi.org/10.3390/su15010138>

Academic Editor: Joana Ferreira

Received: 5 September 2022

Revised: 11 December 2022

Accepted: 14 December 2022

Published: 22 December 2022



Copyright: © 2022 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>).

1. Introduction

Sulphur dioxide (SO₂) is a toxic atmospheric pollutant. It is the major indicator used to monitor air quality and is associated with an increased risk of cardiovascular disease [1]. It can also be oxidised and converted into sulphuric acid mist or sulphate aerosols, leading in turn to the formation of acid rain, which has adverse impacts on human health, building materials, historical sites, and the ecological environment. Because of the negative impacts of SO₂, early detection and close monitoring of ambient SO₂ levels are desirable.

SO₂ can be detected via chemical methods and remote-sensing methods. Chemical methods for the detection of SO₂ concentrations include titration, ion chromatography, calorimetry, mass spectrometry, conductimetry, amperometric detection, flame photometric detection, and turbidimetry. Chemical methods have high accuracy and low detection limits. However, these methods require chemical reagents and cannot provide real-time monitoring results. Remote-sensing methods for monitoring ambient SO₂ concentrations include differential absorption lidar (DIAL), differential optical absorption spectroscopy (DOAS) [2], ultraviolet fluorescence [3], iodine method [4], infrared absorbance [5], and ultraviolet absorbance [6]. Remote-sensing methods have the merits of non-contact implementation and fast speeds. They can be applied to monitor SO₂ gas levels under inconvenient sampling conditions, providing fast detection and continuous monitoring. UV spectrometer and UV camera approaches are two variations of the ultraviolet absorbance method. With the advantage of high spectral resolution, the UV spectrometer approach for SO₂ monitoring was first introduced by Moffat and Millan [7]. Since then, it has been widely applied to the measurement of SO₂ emissions from volcanos and industrial plants [8]. The UV camera approach allows images of certain ranges of wavebands to be captured. As the quantum

efficiency of these cameras has drastically improved, the rising popularity of the UV camera method has enabled high time resolution, allowing transient explosive events to be captured. The captured images provide spatial information, for instance, about shape and topological space. Since this approach provides spatial information and time information at the same time, it can be used to calculate the plume transport velocity [9]. The UV camera method has been successfully implemented for monitoring SO₂ emissions from power plants and industrial stacks [10,11] and even lower SO₂ emissions from ships [12,13].

Khan, et al. [14] indicated overlaps of the ultraviolet absorption band of SO₂ and those of other common gases (e.g., NO₂, O₃) and reported that the absorption coefficient of SO₂ varies with wavelength. However, previous studies of the UV camera approaches have been restricted by limitations such as the use of single-spectrum UV imagery and the modelling of only natural environments (good visibility, bright and uniform sky) while ignoring environmental factors. The systematic modelling correlation between UV absorbance and SO₂ concentration under various environmental conditions, therefore, remains mysterious. Systematic modelling of the relationship between UV absorbance and SO₂ concentration under various environmental conditions has not yet been done. Multispectral imaging was originally developed in the field of remote sensing [15]. In this method, absorption characteristics of the target are obtained at multiple wavelengths. Therefore, multispectral imaging can be used to study the absorption characteristics of SO₂ at various wavelengths. In this study, a model is introduced to reveal the relationship between UV absorbance and SO₂ concentration using multispectral imaging across a range of various environmental conditions, thus filling in this research gap.

2. Methods

2.1. Spectral Wavelengths for Modelling

SO₂ has three main spectral regions of absorption in the near-ultraviolet spectrum, including (1) very weak absorption in the 340 nm to 390 nm range; (2) semi-strong absorption in the 250 nm to 320 nm range; and (3) strong absorption in the 190 nm to 230 nm range [3]. Most UV light in the range of 190 nm to 230 nm is absorbed by atmospheric ozone (O₃). In addition, owing to technical restrictions, the optical devices used for SO₂ measurement, namely the UV camera, UV lens, and UV filter, have low transmission below 250 nm. Therefore, the ideal monitoring wavelength range is 250 nm to 320 nm. For this study, we selected a set of five narrow-band-pass filters manufactured by ASAHI SPECTRA Inc. with different CWLs (centre wavelengths) for the calculation of 10 nm full width at half maximum (FWHM) differences for an array of wavelengths, i.e., 270 nm, 280 nm, 300 nm, 310 nm, and 340 nm, as shown in Figure 1. To be more specific, 270 nm, 280 nm, 300 nm, and 310 nm were the wavelengths within the spectral regions of absorption, whereas 340 nm was a control at which no absorption was indicated.

2.2. UV Camera

The UV camera was one of the key hardware components used in this study, and the accuracy of the experiment was affected by its optical performance. Two major factors were considered, including the quantum efficiency and the read noise. First, the UV camera was required to have a high quantum efficiency in the UV waveband in order to maximise signal under weak UV light intensity. Second, a low noise level in the data recorded by the UV camera was needed to minimise unnecessary measurement errors. The iKon-M934 BU2 was selected as the UV camera for use in this research due to its appropriate wavelength range (from 200 nm to 1000 nm), fast frame rate (up to 4.4 f/s), high quantum efficiency in the near-ultraviolet wavelength range (about 60% at 300 nm), and low noise level (6.2 e[−] @ 1 MHz). The lens used for this camera was a Universe Kogaku UV5035B with a wavelength range of 250 nm to 1000 nm. Its focal length was 50.53 mm ± 5%, and the optical distortion was −0.76% in the diagonal.

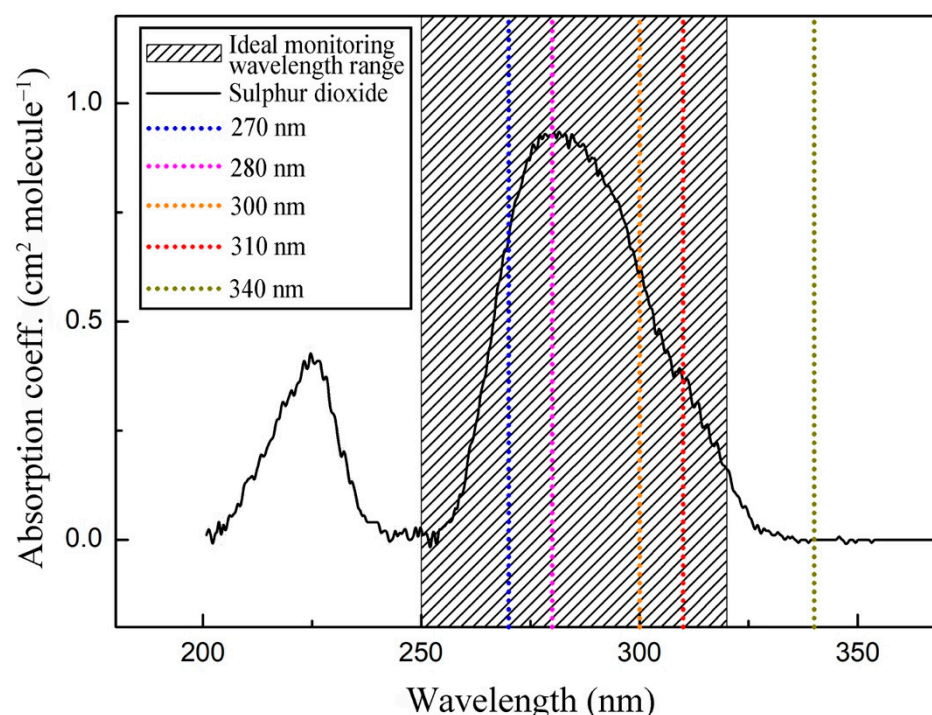


Figure 1. UV absorption spectrum of sulphur dioxide, ideal monitoring wavelength range (i.e., from 250 nm to 320 nm.), and selected wavelengths (i.e., 270 nm, 280 nm, 300 nm, 310 nm, 340 nm).

2.3. Control Set-Up

The relationship between SO₂ concentration and UV absorbance may be affected by various atmospheric parameters, such as humidity, gas flow rate, and temperature [16,17]. To study the influence of environmental factors, experiments have to be conducted with one varying variable while all other variables are kept under control. To achieve this goal, a special device was developed for this study, as shown in Figure 2. The device consisted of a gas concentration and humidity adjuster, a humidity detector, a gas cell, a temperature controller, a pressure controller, a UV light source, an optical fibre, and a tail gas treatment. The light source was a deuterium lamp. The light path was 4.2 metres via multiple reflections in the cell. The SO₂ gas concentration was 2000 ppm. The N₂ gas was 99.999% pure. The liquid in the tail gas treatment was NaHCO₃ (500 mg mL⁻¹).

2.4. Calculation of Absorbance from the UV Camera Images

Absorbance $A(\lambda)$ was the unit used to represent the level of UV light absorbed by a certain SO₂ concentration. The Beer–Lambert law can be used to represent the atmospheric extinction process and infer the gas concentration based on absorption characteristics [18]. The Beer–Lambert law calculations indicated that different concentrations of SO₂ corresponded to different absorbances.

The transmittance T is the ratio of the intensity of transmitted light to the intensity of incident light, as shown in Formula (1).

$$T(\lambda) = \frac{I(\lambda)}{I_o(\lambda)} \quad (1)$$

where $I(\lambda)$ is the transmitted intensity, $I_o(\lambda)$ is the intensity of incident light, and the absorbance, denoted $A(\lambda)$, is as follows:

$$A(\lambda) = \ln\left(\frac{1}{T(\lambda)}\right) = \ln\left(\frac{I_o(\lambda)}{I(\lambda)}\right) \quad (2)$$

The Beer–Lambert law can be shown in Formula (3).

$$I(\lambda) = I_0(\lambda) \exp[\sigma(\lambda)CL] \quad (3)$$

where $\sigma(\lambda)$ is the molar attenuation coefficient, C is the concentration of the gas, and L is the path length of the light beam.

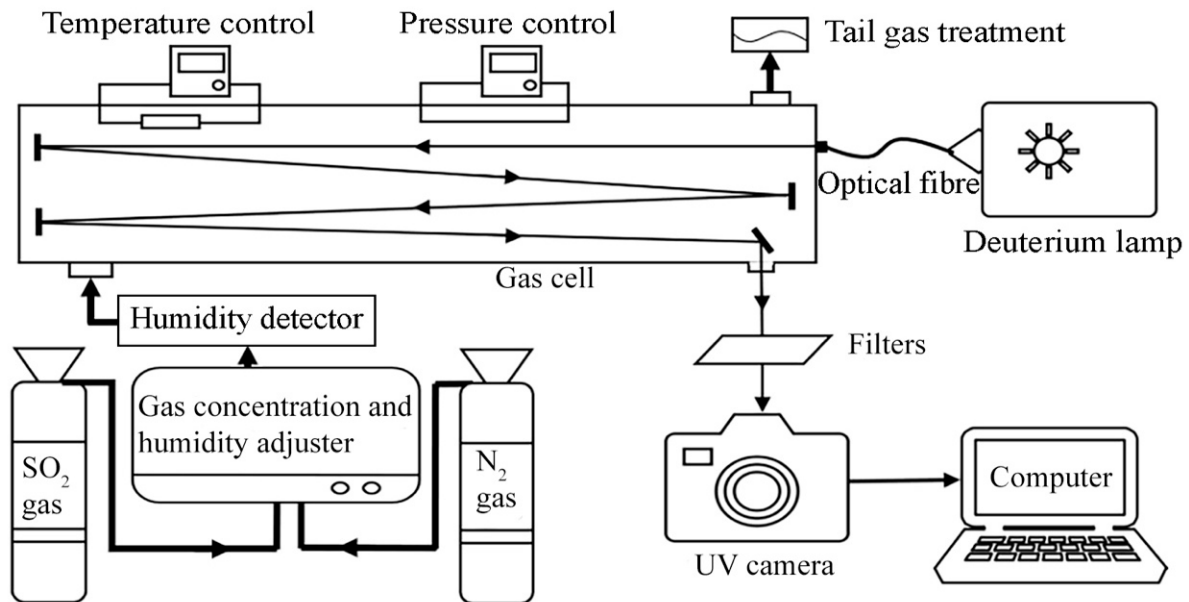


Figure 2. A schematic diagram of the special device designed for this experimental laboratory study. Gases with different SO_2 concentrations and humidities were mixed in the gas adjuster. The mixed gases were then added to the gas cell. Temperature and pressure inside the gas cell were controlled by the temperature controller and the pressure controller. The light source provided simulated sunlight, including light in the UV range. The light subsequently travelled through the gas cell and individual filters, and continuous images were captured by the UV camera placed in front of the cell.

By combining Formulas (2) and (3), the following can be obtained:

$$A(\lambda) = \ln\left(\frac{I_0(\lambda)}{I(\lambda)}\right) = \sigma(\lambda)CL \quad (4)$$

Therefore, concentration C can be calculated using Formula (5):

$$C = \frac{A(\lambda)}{\sigma(\lambda)L} \quad (5)$$

The images taken by the UV camera are presented as Counts (Ct). Counts represent raw digitised data (i.e., no calculations or processing have been applied) from the CCD detector's analogue to digital (A/D) converter. This numerical value can be calculated by many statistics tools, e.g., MATLAB, Microsoft Excel, Minitab, and Python programming. Therefore, $A(\lambda)$ can be calculated using the Ct of the image, while transmission $T(\lambda)$ can then be calculated as follows:

$$T(\lambda) = \frac{Sig(\lambda) - Bg(\lambda)}{Ref(\lambda)} \quad (6)$$

where $Sig(\lambda)$ is the count value of the picture; $Bg(\lambda)$ is the data in uncorrected Counts, acquired in darkness; and $Ref(\lambda)$ is the background corrected incident intensity, which is

normally acquired from the light source without the light being reflected from or passed through the material in the device, i.e., only N₂. Therefore,

$$Ref(\lambda) = Sig(\lambda)' - Bg(\lambda) \quad (7)$$

where $Sig(\lambda)'$ is the signal acquired from the light source without SO₂.

Therefore, the absorbance $A(\lambda)$ captured by the UV camera can be expressed as follows:

$$A(\lambda) = \ln\left(\frac{I_o(\lambda)}{I(\lambda)}\right) = \ln\left(\frac{Ref(\lambda)}{Sig(\lambda) - Bg(\lambda)}\right) = \ln\left(\frac{Sig(\lambda)' - Bg(\lambda)}{Sig(\lambda) - Bg(\lambda)}\right) \quad (8)$$

Figure 3 illustrates how the light source was presented in the UV camera images. As can be seen by comparing the two images in Figure 3, the light passing through SO₂ became weaker, as shown in Figure 3a, while a light spot was visible when the light passed through N₂. Determined through numerical calculation, $Sig(\lambda)'$ is the count value of the light spot in Figure 3b; $Sig(\lambda)$ is the count value of the light spot in Figure 2a. $Bg(\lambda)$ is thus the average count value acquired in the darkness.

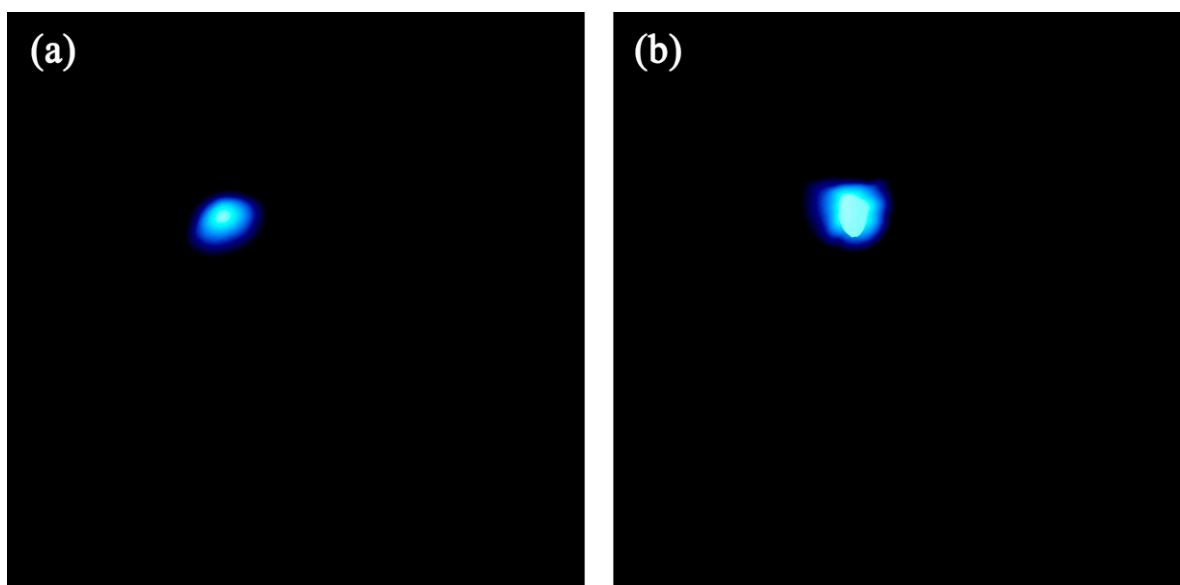


Figure 3. The images of the light source were captured by the UV camera. (a) A light spot image of 1300 ppm of SO₂ in the gas cell. (b) A light spot image of only N₂ in the gas cell. Apart from the gas injected into the container, the other environmental factors remained the same.

3. Quality Assurance of the Control Set-Up

Due to the complexity of the experimental system, quality assurance processes were essential to validate every part of the design and ensure all components were functioning properly [19]. To ensure the accuracy of the results from the device, the following quality assurance procedures were conducted: (1) device stability test; (2) blank control tests, i.e., zero SO₂ concentration and zero light intensity; and (3) repeatability test. These tests are described in the following sections.

3.1. Device Stability Test

The device stability test involved testing the stability of two components, namely the light source and the UV camera. A spectrometer made by Ocean Optics was used to validate the stability of the light source, with continuous samples recorded every five minutes over a period of 125 min. The results shown in Figure 4 indicate that the light source was fairly stable across all samples, having a similar pattern over the whole testing period. A standard deviation was computed for every 5 min interval between 5 and 125 min, giving 25 records

for each wavelength in the range of 200 nm to 400 nm. The maximum standard deviation was 0.4%, observed at 260 nm.

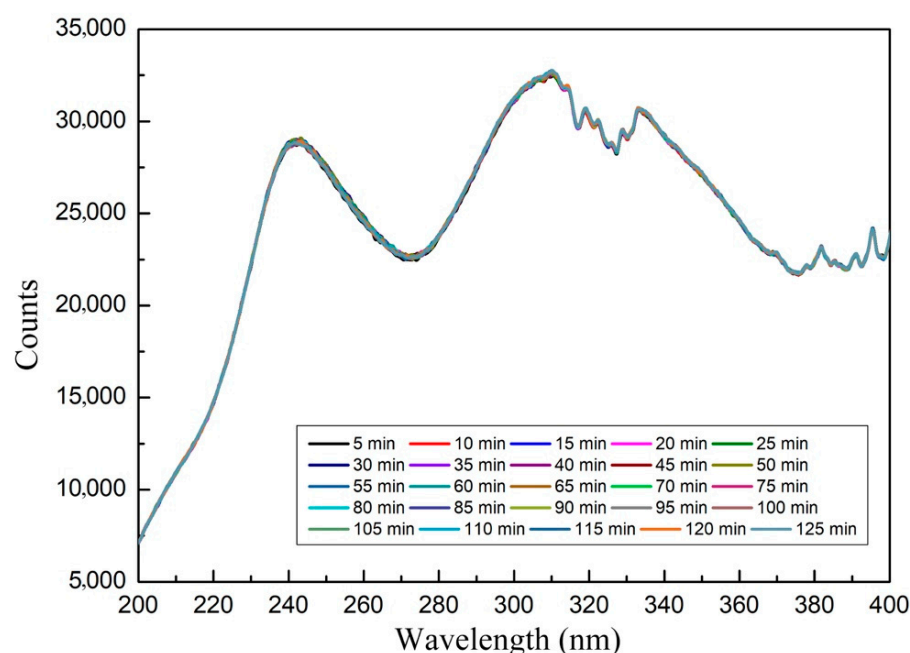


Figure 4. Light source patterns over a period of 125 min (5 min intervals) in the device stability test.

The UV camera stability was tested under control conditions with a 5 min interval between each shot over a test period of 35 min. Test conditions were as follows: 2.56 s exposure time, 1 atm (standard atmosphere), 25 °C, 1200 ppm SO₂ concentration, 0 mL/min gas flow rate, with a 280 nm filter. The absorbance values measured using the UV camera were consistent and showed a similar pattern to that recorded using the Ocean Optics spectrometer, as shown in Figure 5. As such, the device can be regarded as very stable; the relative standard deviation (RSD) of the UV camera was only 6.98%, while the RSD of the spectrometer was 7.41%. This also implies that the UV camera was more stable than the commercial spectrometer in terms of absorbance performance.

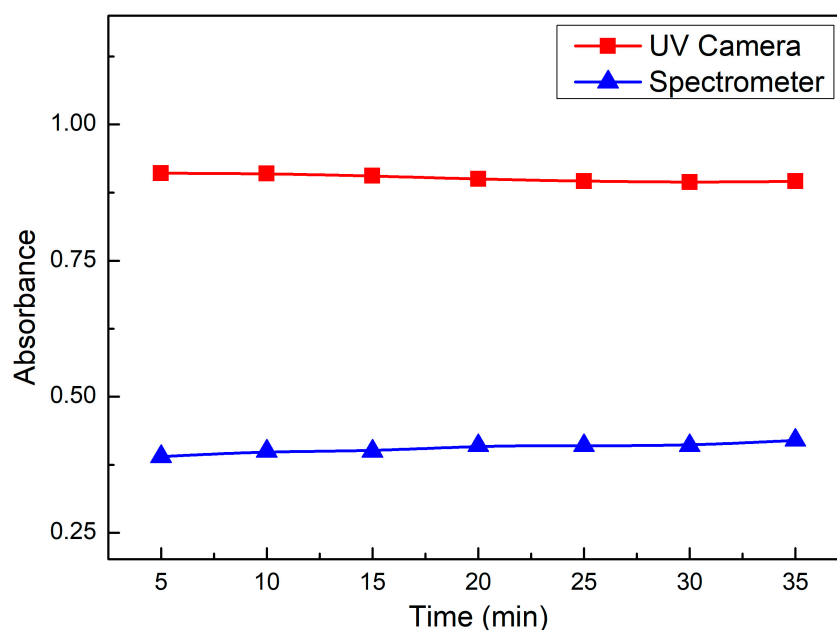


Figure 5. Absorbance results from the UV camera in the device stability test.

3.2. Blank Control Test

The blank control testing involved two tests, i.e., a zero light intensity test and a zero SO₂ concentration test.

First, the zero light intensity test required us to acquire the background (image) of the UV camera, i.e., the uncorrected Counts captured in darkness. Counts are the basic data of the iKon-M934 BU2 camera. The background data are the uncorrected Counts acquired in darkness. Therefore, the true value of an image can be obtained by eliminating the background, as shown in Formula (9):

$$\text{Counts (Corrected)} = \text{Counts} - \text{Background} \quad (9)$$

A set of tests with filters of 270 nm, 280 nm, 300 nm, 310 nm, and 340 nm was conducted 20 times for each wavelength to obtain the backgrounds. Figure 6 shows an example of a background image captured by the UV camera using the 300 nm filter. According to the analysis of these images, the image intensity of the background was consistent, and the variation of all data was only 0.6%.

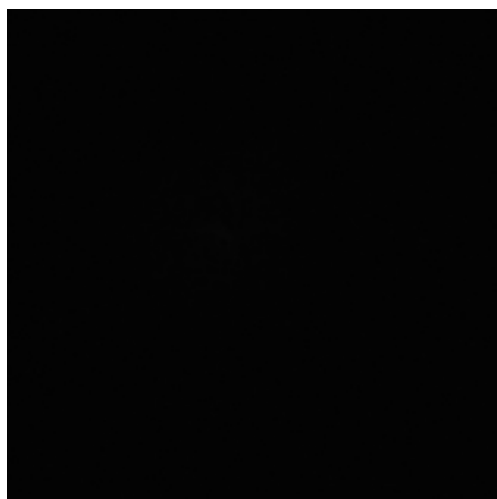


Figure 6. Images were taken by the UV camera in the absence of light to observe the homogeneity of the black brightness.

Second, the zero SO₂ concentration test was conducted by obtaining UV images with zero SO₂ concentration in the gas cell. A set of experimental tests with filters of 270 nm, 280 nm, 300 nm, 310 nm, and 340 nm was conducted with zero SO₂ concentration. In total, 10 images were captured by the UV camera at each wavelength. These experiments were carried out in the laboratory, with the same controlled conditions, i.e., temperature, relative humidity, pressure, gas flow rate, and camera settings, used for each set of data. The blank control data were used as the reference data to calculate the absorbance in the theoretical model.

3.3. Repeatability Test

A repeatability test was carried out to confirm the validity of the similar patterns observed when conducting repeated experiments. Repeatability tests were carried out in a controlled laboratory environment for wavelengths of 270 nm, 280 nm, 300 nm, 310 nm, and 340 nm, and for all SO₂ concentrations from 0 to 1000 ppm, with 10 images shot for each measurement. The tests were categorised into three different groups and validated by repeated experiments. Figure 7 shows an example of repeated experiments for the wavelength of 310 nm. The results showed a consistent pattern with an RSD of only 3.52%.

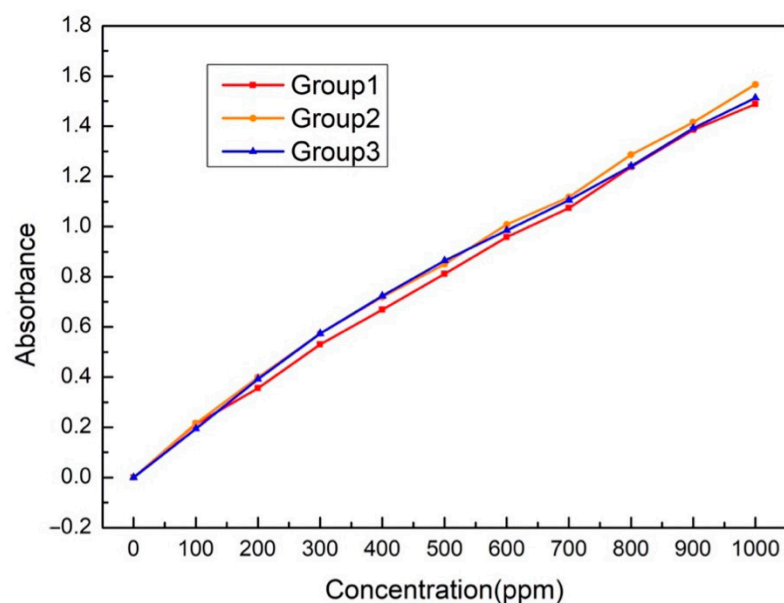


Figure 7. Repeatability experiment results were recorded by the UV camera in the 310 nm waveband.

4. Experiment and Analysis

4.1. Analysis of UV Absorbance by Different SO₂ Concentrations at Multiple UV Wavelengths

A systematic experiment for obtaining the UV absorbance of different SO₂ concentrations at five wavelengths was carried out using filters. The narrow-band-pass filters were 270 nm, 280 nm, 290 nm, 310 nm, and 340 nm. The environmental factors of the experiment are shown in Table 1.

Table 1. Environmental factors and the experimental set-up used in this study.

Items	Values
Narrow-band-pass filters (nm)	270, 280, 300, 310, 340
SO ₂ concentrations (ppm)	Interval = 20 ppm, range = from 0 to 1000
Exposure time (s)	0.2, 1.0, 1.8
Temperature (°C)	25
Items	f16

The absorbance level is graphed against SO₂ concentration in Figure 8. The trend of UV absorbance at 340 nm showed an ideal curve close to zero, implying that SO₂ had no UV absorption at 340 nm, matching the theoretical assumption [3]; therefore, it was removed from the regression model. The UV absorbance at the other four CWLs can be represented by the following regression model:

$$A = aX^2 + bX + c \quad (10)$$

where a , b , and c are the fitting coefficient values as shown in Table 2, A is for the absorbance, and X is for the SO₂ concentration.

Table 2. Fitting coefficients and R² values of the regression models of absorbance level against SO₂ concentration at the wavelengths of 270 nm, 280 nm, 300 nm, and 310 nm.

CWL	a	b	c	R ²
270 nm	-2.6853×10^{-6}	5.7887×10^{-3}	-2.2263×10^{-4}	0.9995
280 nm	-4.1456×10^{-6}	7.5761×10^{-3}	1.0812×10^{-3}	0.9992
300 nm	-1.1977×10^{-6}	4.3508×10^{-3}	2.5618×10^{-2}	0.9995
310 nm	-2.9712×10^{-7}	1.7151×10^{-3}	3.1292×10^{-2}	0.9987

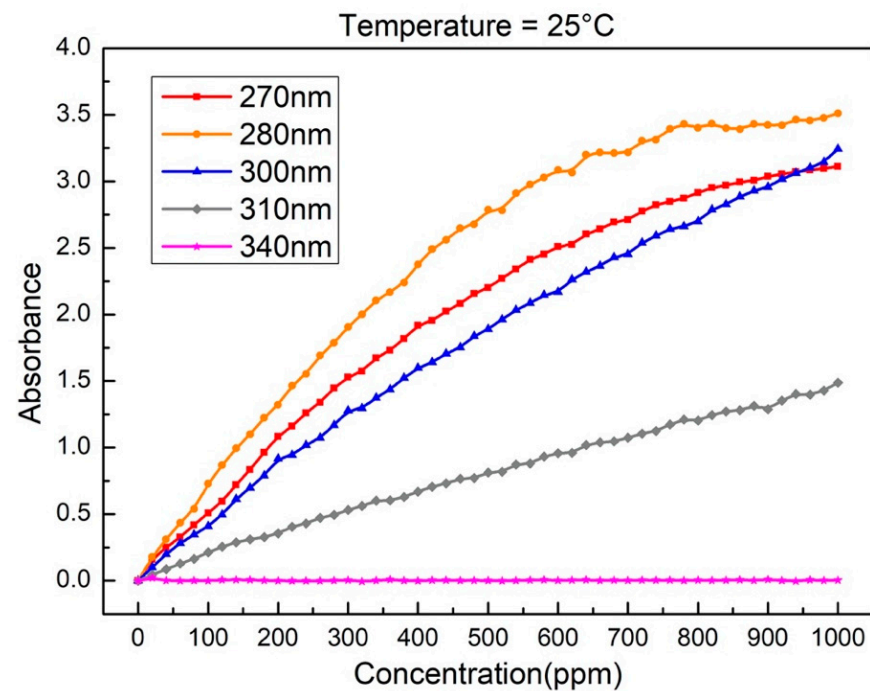


Figure 8. UV absorbance of different SO₂ concentrations at CWLs of 270 nm, 280 nm, 300 nm, 310 nm, and 340 nm below 25 °C.

4.2. The Influence of Gas Flow Rate

The effect of the gas flow rate was tested within the following conditions: a gas flow rate ranging from 100 mL/min to 1000 mL/min with a rate interval of 100 mL/min, a 280 nm filter, a 2.56 s exposure time, 0.5 MPa, a 1200 ppm SO₂ concentration, and 30 °C. Figure 9 shows the results of the gas flow rate effect test. The result was very stable (around 650) with an RMSE of 4.2, implying that the gas flow rate had no apparent effect on SO₂ monitoring.

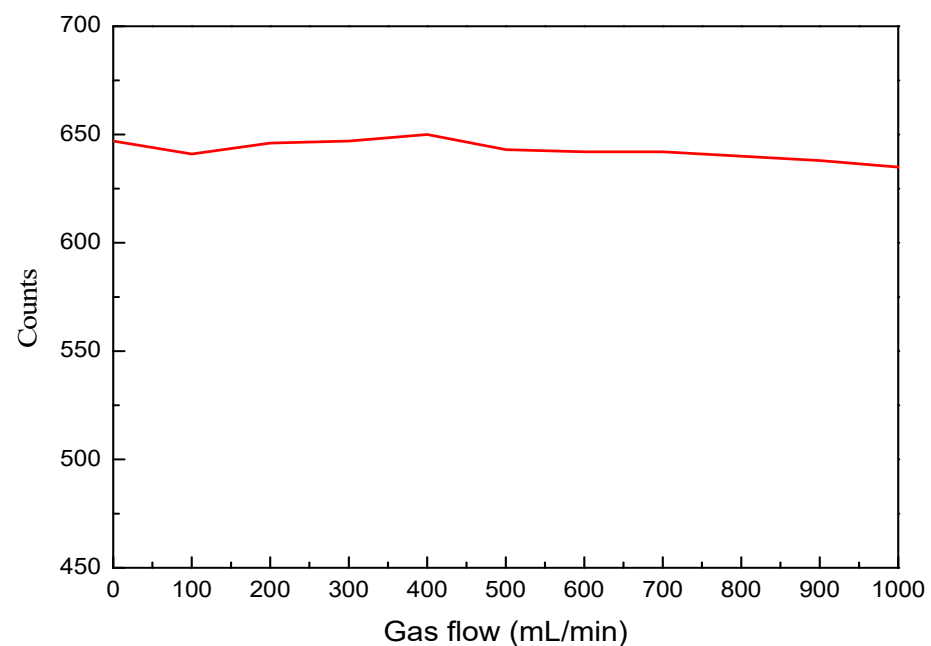


Figure 9. UV absorbance of SO₂ influenced by gas flow rate.

4.3. The Influence of Relative Humidity

The SO₂ absorbance was not significantly affected by the relative humidity, showing fairly stable absorbance values with an average RMSE of 0.0277, as shown in Figure 10. The RSDs of 270 nm, 280 nm, 300 nm, and 310 nm were 1.01%, 0.58%, 0.72%, and 2.77%, respectively. It was concluded that RH is not a considerable factor influencing SO₂ absorbance.

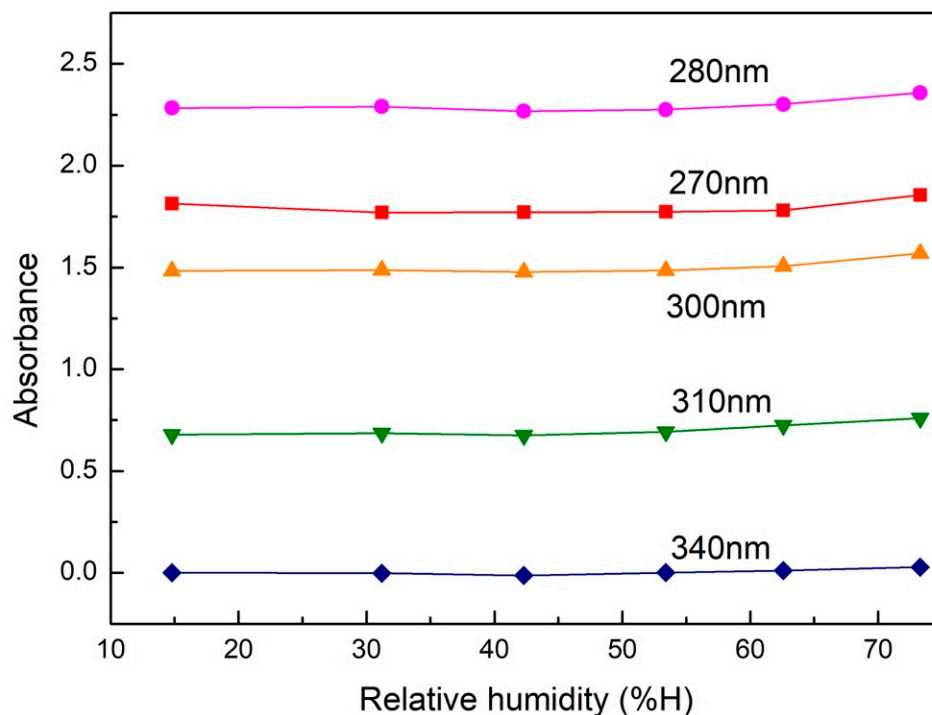


Figure 10. UV absorbance of SO₂ is influenced by relative humidity.

4.4. The Influence of Temperature

To study the effect of temperature effect, the SO₂ absorbance was measured at multiple temperatures: under 5 °C, 15 °C, 25 °C, 35 °C, and 45 °C. Figure 11 illustrates the absorbance of UV light at five different wavebands by SO₂ with a concentration of 500 ppm. The maximum differences in absorbance at 270 nm, 280 nm, 300 nm, and 310 nm were 0.4226, 0.5179, 0.2849, and 0.1349, respectively. The RSDs of 270 nm, 280 nm, 300 nm, and 310 nm were 7.29%, 7.28%, 6.02%, and 7.36%, respectively. The huge difference confirmed that the influence of temperature is highly significant. Additional systematic experiments similar to the previous ones were carried out at 5 °C, 15 °C, 35 °C, and 45 °C, as shown in Figure 12.

4.5. Integrated Look-Up Tables (LUTs) for an Array of Environmental Factors

In the analysis of the experimental results, the gas flow rate and relative humidity were not considered due to their negligible effect on UV absorbance at different SO₂ concentrations. The analysis focused on depicting how the variation of wavelengths and temperatures correlated to UV absorbance at different SO₂ concentrations. As such, look-up tables (LUTs) were developed based on the research data collected in this study. The input parameters were waveband, absorbance, temperature, and distance, while the output parameter was the SO₂ concentration. The resolution of the SO₂ concentration was 20 ppm. The four heat maps of the LUTs are shown in Figure 13.

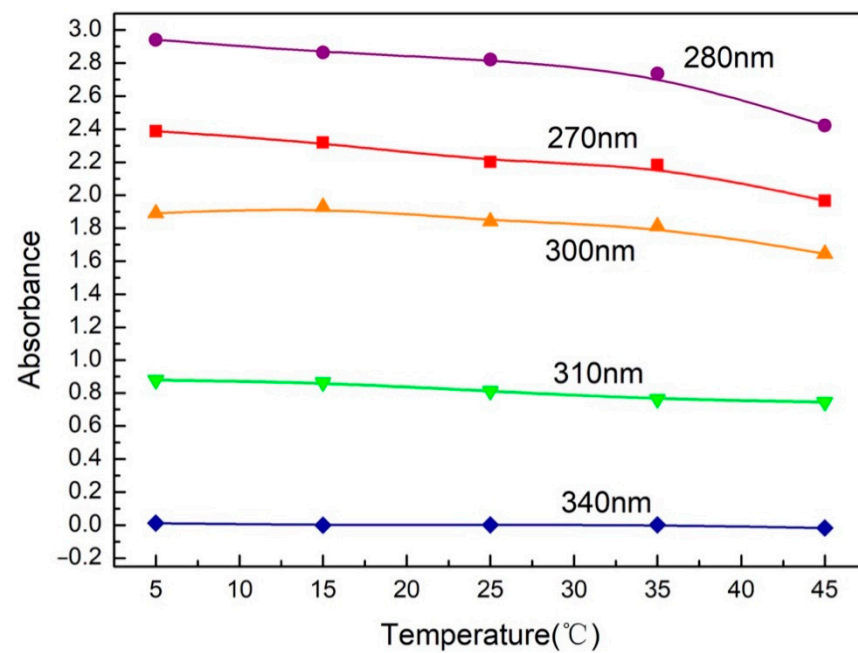


Figure 11. Influence of temperature on the UV absorbance of SO₂ at 500 ppm concentration.

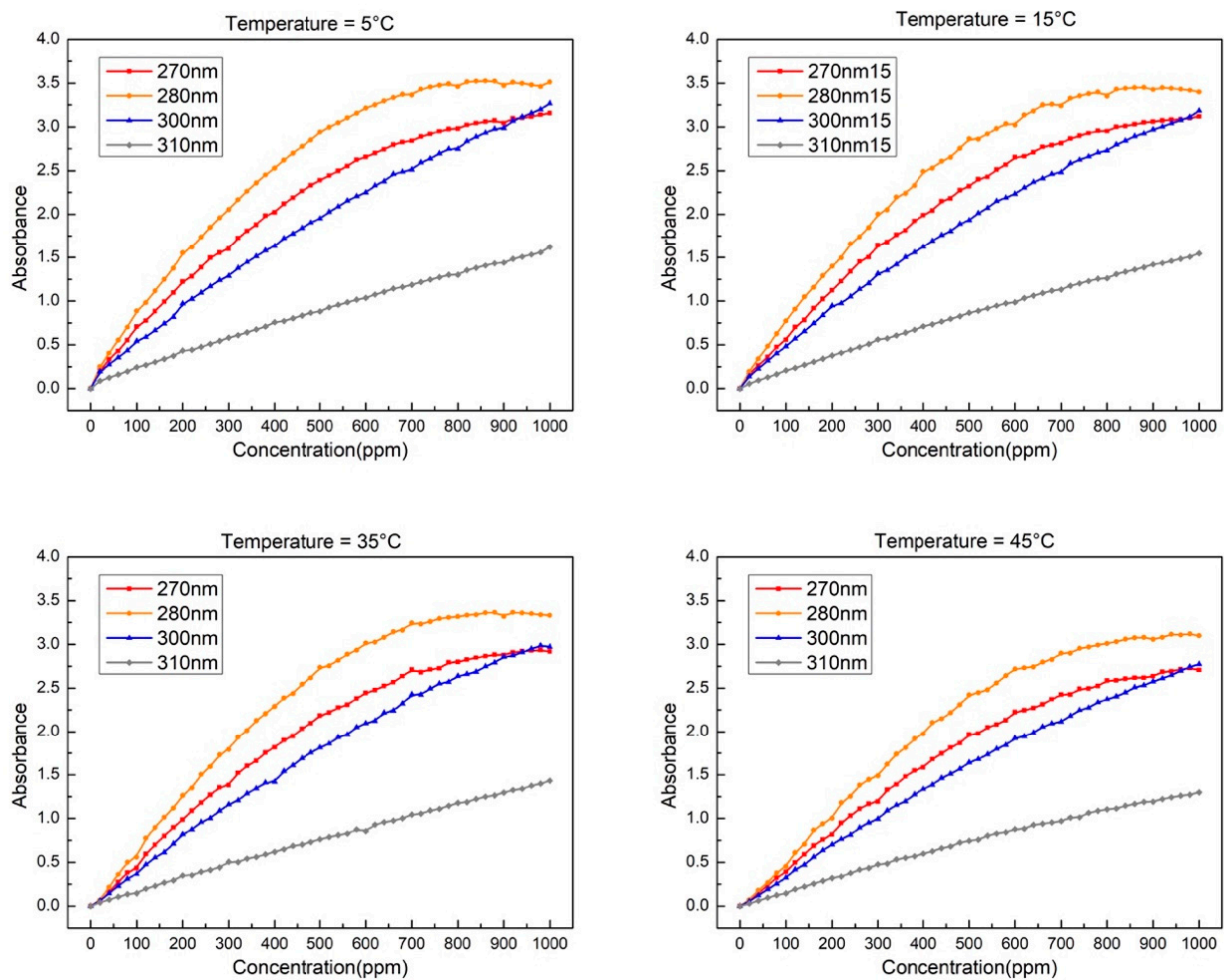


Figure 12. UV absorbance of different SO₂ concentrations at fixed temperatures, i.e., 5 °C, 15 °C, 35 °C, 45 °C, and different wavelengths of 270 nm, 280 nm, 300 nm, and 310 nm.

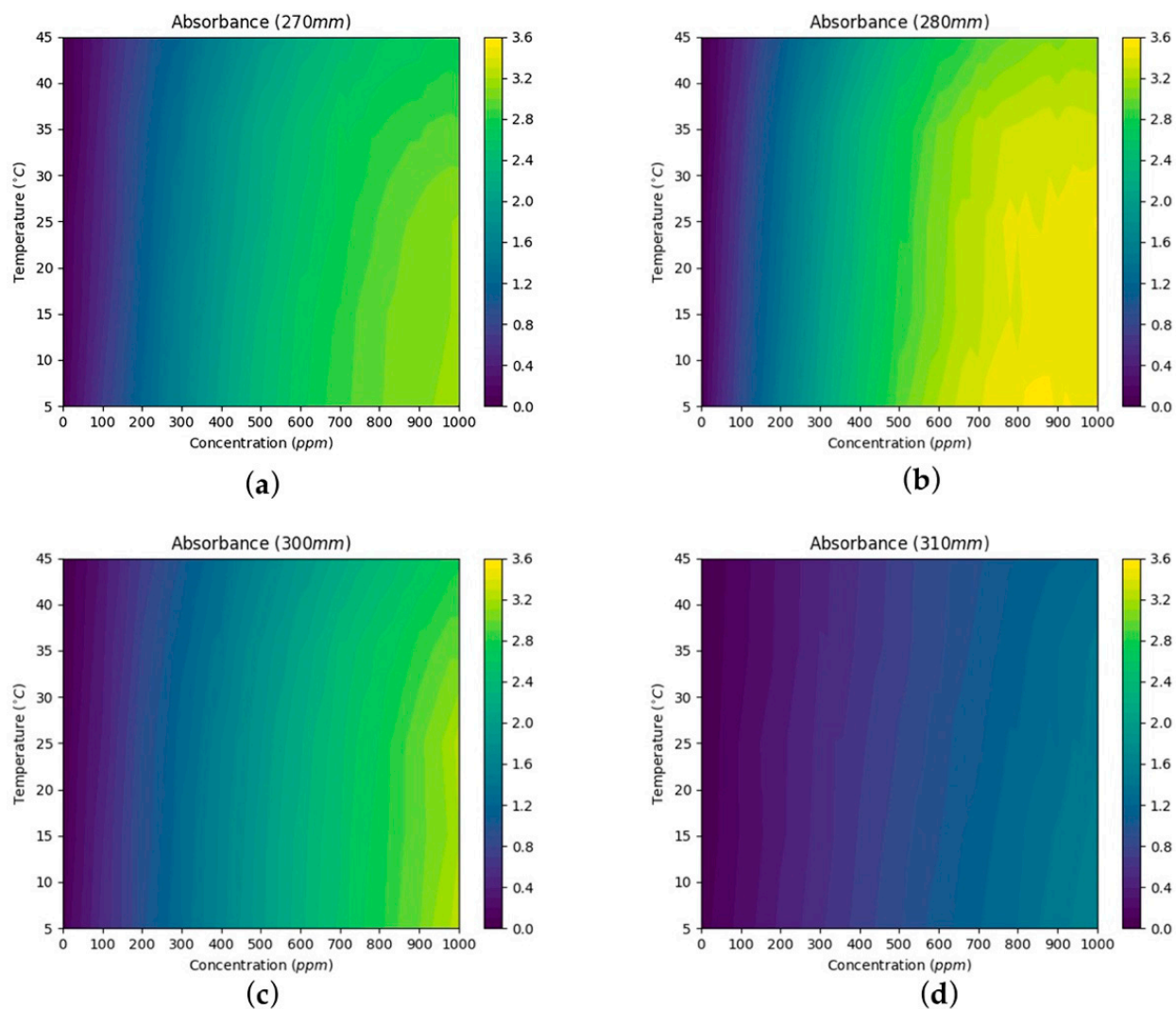


Figure 13. LUTs in the heat map set indicate the relationships between UV absorbance, SO_2 concentration, and other parameters at four UV wavelengths: (a) relationships at the wavelength of 270 nm; (b) relationships at the wavelength of 280 nm; (c) relationships at the wavelength of 300 nm; (d) relationships at the wavelength of 310 nm.

4.6. Noise Removal for LUTs

Smoothing is a commonly used method to remove noise from data [20,21]. In view of the measurement uncertainties in the original data, noise removal for the LUTs was implemented via quadratic polynomial fitting at each wavelength to minimise the adverse measurement effect. The fitting coefficients and R^2 values are listed in Table 3.

The standard deviation (SD) value and the absolute value of the residuals between the original measured data and the fitted value of each band, each wavelength, and each temperature were calculated. The maximum SD for temperature was calculated and is shown in Table 4. The maximum SD of the regression model was only 0.086. The absolute values of the residuals of each temperature were classified according to Jenks natural breaks, which is a data-clustering method used in cartography and statistics. The Jenks natural breaks method was first introduced by Jenks [22]. It determines the best arrangement of values into different classes. The results are shown in Figure 14 and showed that the absolute values were small. Therefore, both the SDs and the absolute values of the residuals between the original measured data and fitted values were small, indicating that this quadratic polynomial fitted model was acceptable. Figure 15 illustrates the LUTs after smoothing by adopting values from the quadratic polynomial regression models.

Table 3. Fitting coefficients and R^2 values of the regression models of absorbance level at different SO_2 concentrations at temperatures of 5 °C, 15 °C, 25 °C, 35 °C, and 45 °C and wavelengths of 270 nm, 280 nm, 300 nm, and 310 nm.

Temperature	CWL	a	b	c	R^2
5 °C	270 nm	-3.1501×10^{-6}	6.1824×10^{-3}	7.6253×10^{-2}	0.9995
	280 nm	-4.6217×10^{-6}	7.9696×10^{-3}	9.9150×10^{-2}	0.9995
	300 nm	-1.2499×10^{-6}	4.3789×10^{-3}	9.1311×10^{-2}	0.9994
	310 nm	-3.2138×10^{-7}	1.8563×10^{-3}	4.8064×10^{-2}	0.9994
15 °C	270 nm	-3.1394×10^{-6}	6.2253×10^{-3}	6.4294×10^{-3}	0.9996
	280 nm	-4.3782×10^{-6}	7.7215×10^{-3}	3.8784×10^{-2}	0.9994
	300 nm	-1.4124×10^{-6}	4.5101×10^{-3}	5.0661×10^{-2}	0.9997
	310 nm	-3.2119×10^{-7}	1.8342×10^{-3}	1.9879×10^{-2}	0.9998
25 °C	270 nm	-2.6853×10^{-6}	5.7887×10^{-3}	-2.2263×10^{-4}	0.9995
	280 nm	-4.1456×10^{-6}	7.5761×10^{-3}	1.0812×10^{-3}	0.9992
	300 nm	-1.1977×10^{-6}	4.3508×10^{-3}	2.5618×10^{-2}	0.9995
	310 nm	-2.9712×10^{-7}	1.7151×10^{-3}	3.1292×10^{-2}	0.9987
35 °C	270 nm	-2.8896×10^{-6}	5.9008×10^{-3}	-7.0890×10^{-2}	0.9995
	280 nm	-4.2674×10^{-6}	7.6865×10^{-3}	-9.3008×10^{-2}	0.9992
	300 nm	-1.2219×10^{-6}	4.2704×10^{-3}	-2.1961×10^{-2}	0.9995
	310 nm	-1.7656×10^{-7}	1.5844×10^{-3}	1.2982×10^{-2}	0.9993
45 °C	270 nm	-2.3689×10^{-6}	5.1818×10^{-3}	-7.6330×10^{-2}	0.9992
	280 nm	-3.4423×10^{-6}	6.6780×10^{-3}	-1.2121×10^{-1}	0.9987
	300 nm	-1.0131×10^{-6}	3.8102×10^{-3}	-2.8500×10^{-2}	0.9998
	310 nm	-3.8191×10^{-7}	1.6842×10^{-3}	-5.4825×10^{-3}	0.9996
5 °C	270 nm	-3.1501×10^{-6}	6.1824×10^{-3}	7.6253×10^{-2}	0.9995
	280 nm	-4.6217×10^{-6}	7.9696×10^{-3}	9.9150×10^{-2}	0.9995
	300 nm	-1.2499×10^{-6}	4.3789×10^{-3}	9.1311×10^{-2}	0.9994
	310 nm	-3.2138×10^{-7}	1.8563×10^{-3}	4.8064×10^{-2}	0.9994

Table 4. Maximum standard deviations of the regression models for each temperature.

Temperature (°C)	5	15	25	35	45
Max SD	0.065	0.052	0.056	0.066	0.086

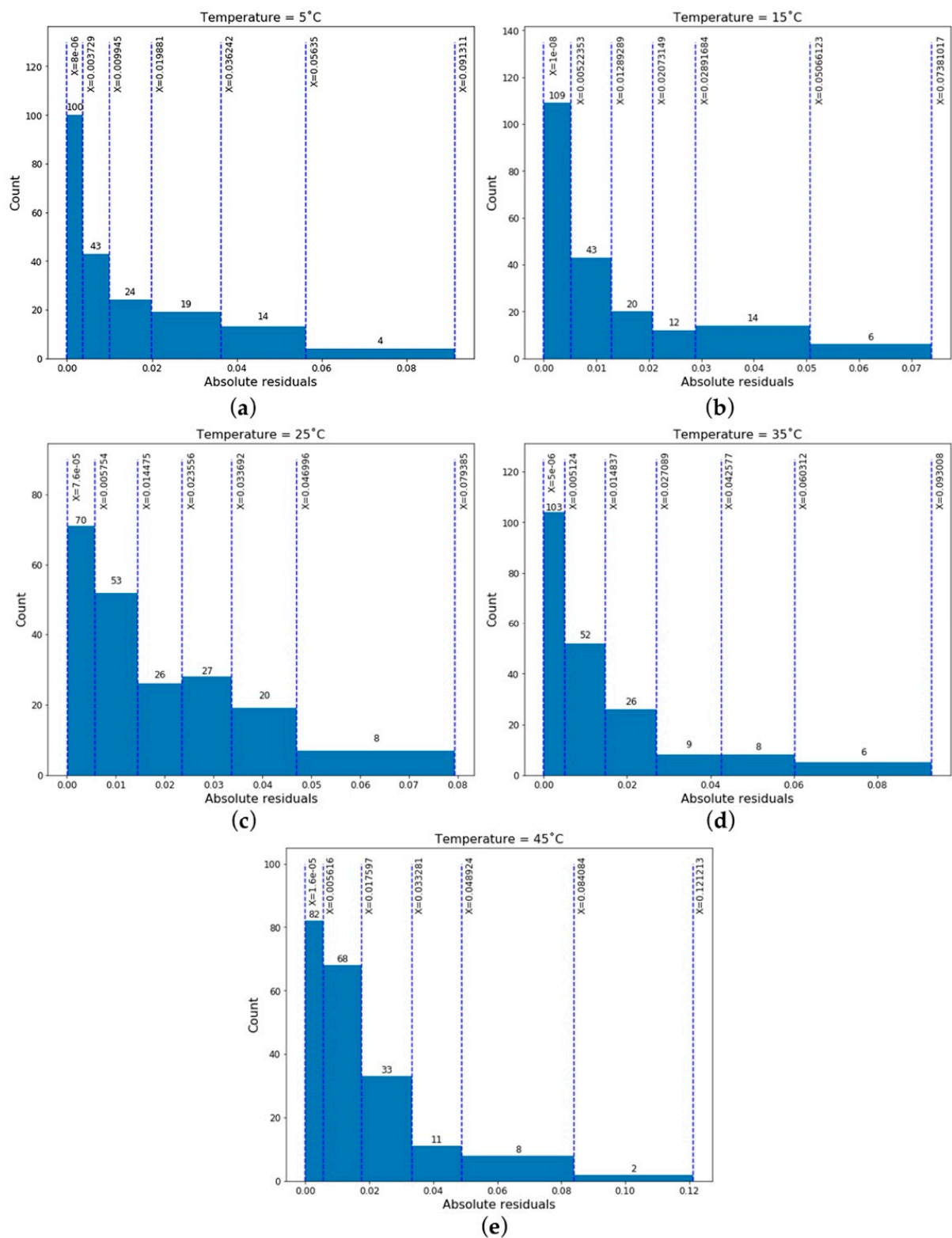


Figure 14. Jenks natural breaks results for absolute values of the residuals between original measured data and fitted values: (a) temperature of 5 °C; (b) temperature of 15 °C; (c) temperature of 25 °C; (d) temperature of 35 °C; (e) temperature of 45 °C.

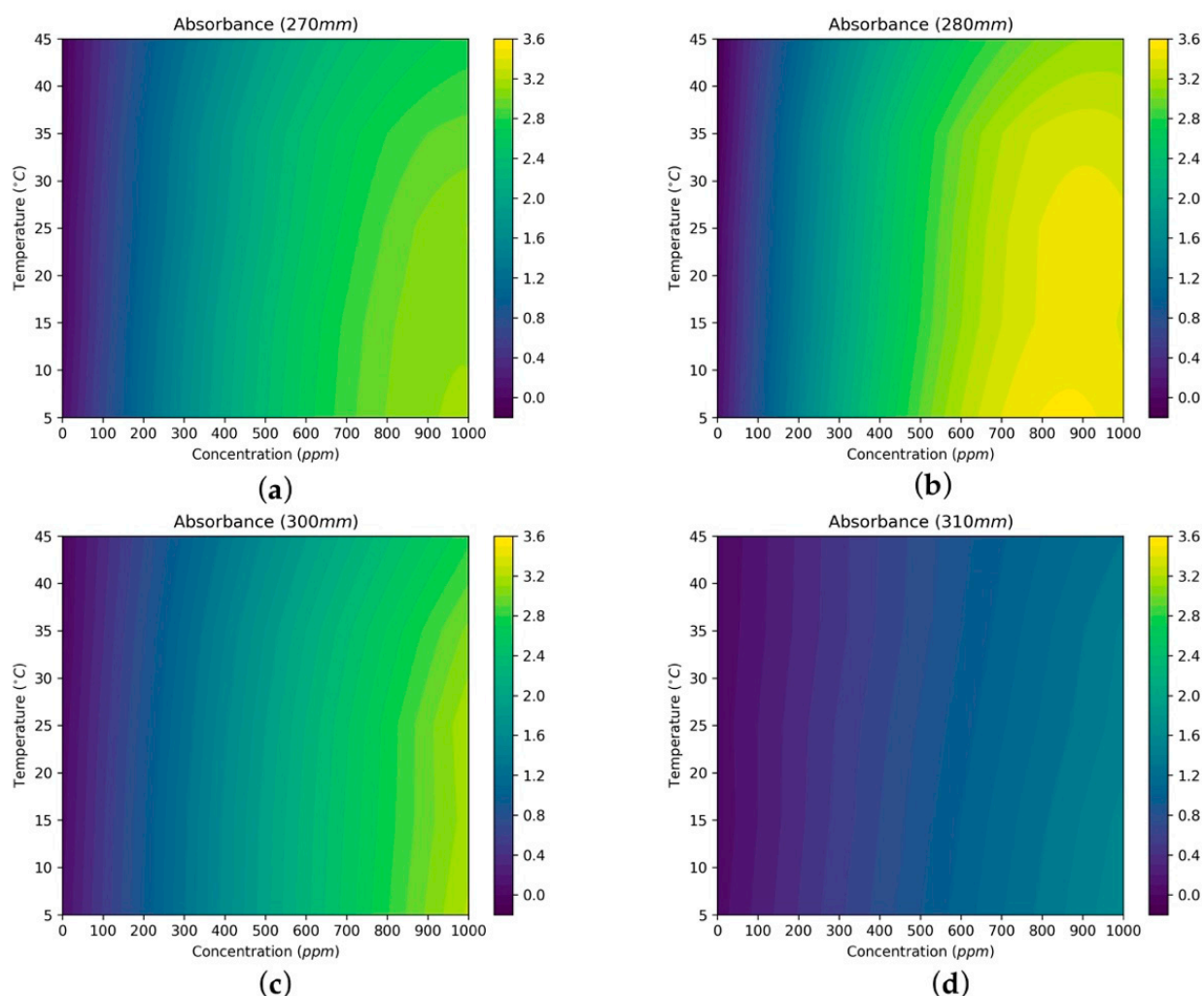


Figure 15. Smoothed LUTs of the relationships between UV absorbance, SO_2 concentration, and other parameters in four UV bands, presented as a heat map set: (a) relationship at the wavelength at 270 nm; (b) relationship at the wavelength at 280 nm; (c) relationship at the wavelength at 300 nm; (d) relationship at the wavelength at 310 nm.

5. Conclusions

Using a multispectral imaging method from the field of remote sensing, the relationships between UV absorbance and SO_2 concentration at multiple UV wavelengths (270 nm, 280 nm, 300 nm, 310 nm, 340 nm) and temperatures (5 °C, 15 °C, 25 °C, 35 °C, 45 °C) were demonstrated via UV camera monitoring. Based on a study of previous literature, a UV range of 250 nm to 320 nm was selected as suitable to illustrate the association of UV absorbance and SO_2 concentration. In order to validate the purpose-built experimental set-up for the control of various environmental factors, including a selected UV camera, UV lens, UV narrow-band-pass filters, a temperature controller, a pressure controller, and a gas concentration and humidity adjuster, quality assurance processes were implemented to ensure the reliability of the experimental results before conducting the tests. It was observed that the light source and the UV camera were fairly stable; in fact, the UV camera performed 5.8% better than the Ocean Optics spectrometer. The intensity of the background images captured by the UV camera was very consistent, with less than a 0.6% standard deviation. The measurements remained the same for each controlled environmental condition, confirming a robust design with only 3.52% RSD in the repeatability test.

The independent variables, i.e., temperature, pressure, relative humidity, gas flow rate, five selected wavelengths, and the SO_2 concentration, were controlled inside this tailor-

made environment. Gas flow rate (from 0 mL/min to 1000 mL/min) and relative humidity (from 14.8% to 73.3%) were observed to have no significant impact on the UV absorbance at different SO₂ concentrations. Temperature and SO₂ concentration exerted substantial influence on UV absorbance, contributing varying effects at different wavelengths, i.e., 270 nm, 280 nm, 300 nm, and 310 nm. The level of UV absorbance remained unchanged at 340 nm, such that we concluded there was no UV absorption by SO₂ at the wavelength of 340 nm. The UV absorbances of four other SO₂ concentrations at wavelengths of 270 nm, 280 nm, 300 nm, and 310 nm were further investigated under the varying temperatures of 5 °C, 15 °C, 25 °C, 35 °C, and 45 °C in 20 ppm SO₂ concentration intervals. The constructed look-up tables (LUTs) showed the relationship between UV absorbance and SO₂ concentration under the influence of various parameters at four UV wavelengths. These results were smoothed by quadratic polynomial fitting. The maximum standard deviation of the regression model was only 0.086. The absolute values of residuals between the original models and the fitted models were analysed using Jenks natural breaks and were determined to be very small. The smoothed LUTs had reduced uncertainties compared to the original model. These models could be applied to future quantification of SO₂ concentration via the UV absorbance method.

Author Contributions: Conceptualisation, Z.L., M.S.W. and K.L.; methodology, Z.L., M.S.W. and K.L.; writing—original draft preparation, K.L.; writing—review and editing, M.S.W.; supervision, Z.L. and M.S.W.; project administration, Z.L.; funding acquisition, Z.L. and M.S.W. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by Hong Kong Environment & Conservation Fund (ECF), grant number 2016-48. M.S. Wong thanks the funding support from the General Research Fund (Grant No. 15603920 and 15609421) and the Collaborative Research Fund (Grant No. C5062-21GF and C7064-18GF) from the Research Grants Council, Hong Kong, China.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Supporting data of Figures 4, 5 and 7 to Figure 15 can be found at the website <https://osf.io/ztrbe/> accessed on 20 April 2022.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Sunyer, J.; Ballester, F.; Tertre, A.L.; Atkinson, R.; Ayres, J.G.; Forastiere, F.; Forsberg, B.; Vonk, J.M.; Bisanti, L.; Tenías, J.M. The association of daily sulfur dioxide air pollution levels with hospital admissions for cardiovascular diseases in Europe (The Aphea-II study). *Eur. Heart J.* **2003**, *24*, 752–760. [CrossRef] [PubMed]
2. Weibring, P.; Edner, H.; Svanberg, S.; Cecchi, G.; Pantani, L.; Ferrara, R.; Caltabiano, T. Monitoring of volcanic sulphur dioxide emissions using differential absorption lidar (DIAL), differential optical absorption spectroscopy (DOAS), and correlation spectroscopy (COSPEC). *Appl. Phys. B Lasers Opt.* **1998**, *67*, 419. [CrossRef]
3. Okabe, H.; Splitstone, P.L.; Ball, J.J. Ambient and source SO₂ detector based on a fluorescence method. *J. Air Pollut. Control Assoc.* **1973**, *23*, 514–516. [CrossRef]
4. Schiavon, G.; Zotti, G.; Toniolo, R.; Bontempelli, G. Amperometric monitoring of sulphur dioxide in liquid and air samples of low conductivity by electrodes supported on ion-exchange membranes. *Analyst* **1991**, *116*, 797–801. [CrossRef]
5. Clarisse, L.; Hurtmans, D.; Clerbaux, C.; Hadji-Lazaro, J.; Ngadi, Y.; Coheur, P.-F. Retrieval of sulphur dioxide from the infrared atmospheric sounding interferometer (IASI). *Atmos. Meas. Tech.* **2012**, *5*, 581–594. [CrossRef]
6. Bluth, G.; Shannon, J.; Watson, I.; Prata, A.; Realmuto, V. Development of an ultra-violet digital camera for volcanic SO₂ imaging. *J. Volcanol. Geotherm. Res.* **2007**, *161*, 47–56. [CrossRef]
7. Moffat, A.J.; Millan, M.M. The applications of optical correlation techniques to the remote sensing of SO₂ plumes using sky light. *Atmos. Environ.* **1971**, *5*, 677–690. [CrossRef] [PubMed]
8. Galle, B.; Oppenheimer, C.; Geyer, A.; McGonigle, A.J.; Edmonds, M.; Horrocks, L. A miniaturised ultraviolet spectrometer for remote sensing of SO₂ fluxes: A new tool for volcano surveillance. *J. Volcanol. Geotherm. Res.* **2003**, *119*, 241–254. [CrossRef]
9. Kern, C.; Werner, C.; Elias, T.; Sutton, A.J.; Lübcke, P. Applying UV cameras for SO₂ detection to distant or optically thick volcanic plumes. *J. Volcanol. Geotherm. Res.* **2013**, *262*, 80–89. [CrossRef]
10. Nadeau, P.A. Ultraviolet Digital Imaging of Volcanic Plumes: Implementation and Application to Magmatic Processes at Basaltic Volcanoes. Ph.D. Thesis, Michigan Technological University, Houghton, MI, USA, 2011.

11. Nisulescu, C.; Ionel, I.; Calinoiu, D. New methods for determination SO₂ emissions. In Proceedings of International Conference Integrated Systems for Agro Food Production, SIPA, Sibiu, Romania, 26–29 September 2013; pp. 10–12.
12. Berg, N.; Mellqvist, J.; Jalkanen, J.; Balzani, J. Ship emissions of SO₂ and NO₂: DOAS measurements from airborne platforms. *Atmos. Meas. Tech.* **2012**, *5*, 1085–1098. [[CrossRef](#)]
13. Prata, A. Measuring SO₂ ship emissions with an ultraviolet imaging camera. *Atmos. Meas. Tech.* **2014**, *7*, 1213–1229. [[CrossRef](#)]
14. Khan, S.; Newport, D.; Le Calvé, S. Gas Detection Using Portable Deep-UV Absorption Spectrophotometry: A Review. *Sensors* **2019**, *19*, 5210. [[CrossRef](#)] [[PubMed](#)]
15. Caballero, D.; Calvini, R.; Amigo, J.M. Hyperspectral imaging in crop fields: Precision agriculture. In *Data Handling in Science and Technology*; Elsevier: Amsterdam, The Netherlands, 2020; Volume 32, pp. 453–473.
16. Li, X.-X.; Wang, Y.; Xu, P.-P.; Zhang, Q.-Z.; Nie, K.; Hu, X.; Kong, B.; Li, L.; Chen, J. Effects of temperature and wavelength choice on in-situ dissolution test of Cimetidine tablets. *J. Pharm. Anal.* **2013**, *3*, 71–74. [[CrossRef](#)] [[PubMed](#)]
17. Wittrock, F.; Oetjen, H.; Richter, A.; Fietkau, S.; Medeke, T.; Rozanov, A.; Burrows, J. MAX-DOAS measurements of atmospheric trace gases in Ny-Ålesund-Radiative transfer studies and their application. *Atmos. Chem. Phys.* **2004**, *4*, 955–966. [[CrossRef](#)]
18. Platt, U.; Stutz, J. Differential absorption spectroscopy. In *Differential Optical Absorption Spectroscopy*; Springer: Berlin/Heidelberg, Germany, 2008; pp. 135–174.
19. Taylor, J.K. *Quality Assurance of Chemical Measurements*; CRC Press: Boca Raton, FL, USA, 1987.
20. Madden, H.H. Comments on the Savitzky-Golay convolution method for least-squares-fit smoothing and differentiation of digital data. *Anal. Chem.* **1978**, *50*, 1383–1386. [[CrossRef](#)]
21. Guiñón, J.L.; Ortega, E.; García-Antón, J.; Pérez-Herranz, V. Moving average and Savitzki-Golay smoothing filters using Mathcad. *Pap. ICEE* **2007**, *2007*, 1–4.
22. Jenks, G.F. The Data Model Concept in Statistical Mapping. *Int. Yearb. Cartogr.* **1967**, *7*, 186–190.

Disclaimer/Publisher's Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.