Scientific Research Publishing

Open Journal of Air Pollution, 2026, 15(2), 48-58
https://www.scirp.org/journal/ojap
ISSN Online: 2169-2661
ISSN Print: 2169-2653

Optimization of UV-Vis Spectrophotometer (OCaPI) Parameters for Measuring the pH and pCO_2 of the Ocean Carbonate System in Seawater to Assess Ocean Acidification (Mediterranean Sea)

Samba Alarba Barry[1*], Cellou Kanté[1], Adama Moussa Sakho[2], Anne-Cécile Ribou[3], Véronique Guglielmi[3], Mamadou Madaniou Sow[1]

[1]Laboratory Techniques Department, Higher Institute of Technology, Mamou, Guinea
[2]Physics Department, Gamal Abdel Nasser University, Conakry, Guinea
[3]Chemistry Department, University of Perpignan Via Domitia, Perpignan, France
Email: *sab.istmamou86@gmail.com

How to cite this paper: Barry, S.A., Kanté, C., Sakho, A.M., Ribou, A.-C., Guglielmi, V. and Sow, M.M. (2026) Optimization of UV-Vis Spectrophotometer (OCaPI) Parameters for Measuring the pH and pCO_2 of the Ocean Carbonate System in Seawater to Assess Ocean Acidification (Mediterranean Sea). *Open Journal of Air Pollution*, **15**, 48-58.
https://doi.org/10.4236/ojap.2026.152003

Received: March 27, 2026
Accepted: May 25, 2026
Published: May 28, 2026

Abstract

Automating the measurement of carbonate system parameters is essential for improving our understanding of biogeochemical processes in marine regions. The portable OCaPI (Ocean Carbon Parameters Instrument) is designed to perform simultaneous and accurate measurements of hydrogen ion concentration (pH) and partial pressure of carbon dioxide (pCO_2)[1] in the ocean environment. Optimizing the parameters of the UV-Vis spectrophotometer (integration time, scan-to-average, boxcar) facilitates the quantification of ocean acidification, with significantly improved measurement accuracy and reliability. The results obtained are consistent with existing techniques and offer a simplified approach to data collection, even under challenging conditions. This work, based on design principles, performance, and preliminary results obtained in the Mediterranean Sea, paves the way for the integration of these optimized techniques into long-term monitoring programs. This will contribute to a better understanding of the impacts of climate change on marine ecosystems and to improved management in the face of ocean acidification.

Keywords

Optimization, OCaPI, Carbonate System, Acidification, Ocean

---

[1] OCaPI: ocean carbon parameters instrument; pH: hydrogen ion concentration; pCO_2: partial pressure of carbon dioxide.

1. Introduction

Assessing the hydrogen ion concentration and the partial pressure of carbon dioxide in seawater is critical for analyzing marine ecosystems and ocean acidification. Optimizing the parameters of the UV-Vis spectrophotometer, particularly for the OCaPI instrument, is essential to ensure the accuracy and reliability of measurements. pH and pCO_2 are crucial parameters of marine carbonate chemistry, which modulate biological and geochemical processes in the oceans [1].

This research demonstrates that integration times of 45,000 µs and 25,000 µs microseconds for pH and pCO_2, respectively, yield reliable results. Improving spectral resolution was made possible by using a 30-point Scan to Average and a 5-point Boxcar, which are essential for reducing background noise. By carefully adjusting these parameters, we gained a better understanding of pH and pCO_2 fluctuations in the oceans, as well as their impacts on climate and marine biodiversity.

Ultimately, collecting accurate information on these variables allows us not only to assess the current state of the oceans but also to predict the future effects of climate change [2] [3].

The study of carbonate system parameters in marine ecosystems is crucial for understanding the effects of environmental changes on the chemical composition of seawater, particularly in the context of increasing acidification linked to rising atmospheric CO_2 levels. This research aims to establish a standardized procedure for measuring these parameters and to contribute to the development of specific standards for seawater analysis [4]-[7].

pH, a key indicator of acidity, influences fundamental biological and chemical processes such as nutrient availability and the metabolism of sensitive organisms like corals and mollusks. At the same time, pCO_2 also plays a major role in the carbon cycle by altering the oceans' ability to absorb atmospheric CO_2, which has direct implications for global warming [1]-[3].

Monitoring these parameters not only allows us to assess the health of marine ecosystems but also to feed into climate models and anticipate the consequences of global changes on biodiversity. Processes such as photosynthesis, respiration, and food chain productivity also depend on them [1] [3] [5] [7].

Accurate measurement, using methods such as UV-Visible spectrophotometry, is therefore crucial for assessing the impact of human activities and for developing strategies for the sustainable management of ocean resources.

2. Materials and Methods

The use of UV-Vis spectrophotometry for these measurements represents an innovative approach that, when properly optimized, can provide accurate and instantaneous data. The experimental methodology adopted for optimizing the parameters of the UV-Vis spectrophotometer aims to ensure a high degree of accuracy in assessing ocean acidification.

The first step involved configuring the spectrophotometer (OCaPI), ensuring that a precise calibration was performed using buffer solutions of known pH to establish a solid reference point. Experimental conditions were standardized, which helped reduce fluctuations caused by external factors.

Optimizing the spectrophotometer's technical parameters (**Figure 9(b)**) is critical to ensuring the precision and accuracy of the results [8]-[12].

Seawater samples were collected in the western Mediterranean in November 2023. Samples were taken at depths ranging from 0 to 10 meters. The environmental conditions observed included a temperature range of 13˚C to 18˚C and a salinity range of 35 to 40 mg/L.

Optimization focuses on three parameters: integration time, Scan to Average, and Boxcar.

2.1. Integration Time

This time, which represents the duration during which the signal is acquired, has a direct impact on the accuracy and sensitivity of the measurements.

The length of the tube (10 cm) was adjusted to match that of the thermostat (18 cm); subsequently, it became necessary to optimize the integration times.

1) pH: Intensity spectra were recorded at seawater pump speeds of 600, a scan-to-average of 30, a boxcar of 5, and integration times of 12,000 to 100,000 µs (**Figure 1**).

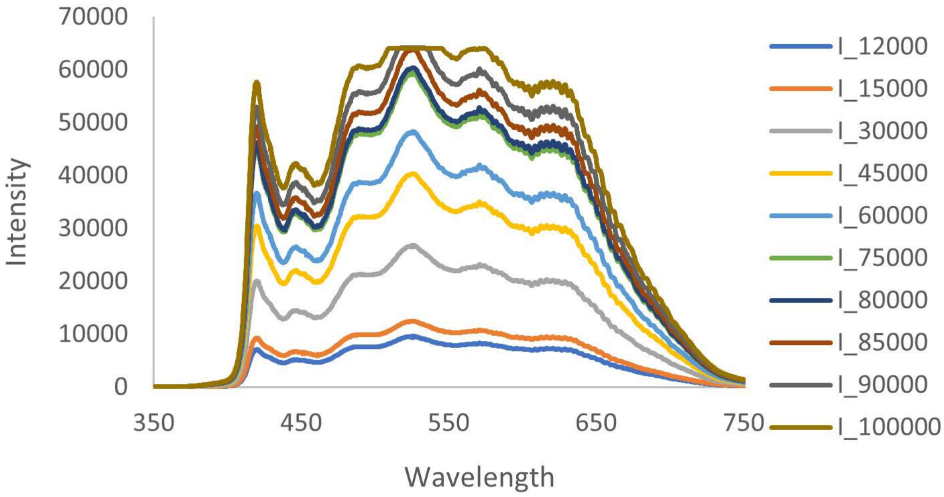


Figure 1. Intensity spectrum of measurements taken with the engine off (seawater pump speed at 600, Scan to Average 30, Boxcar 5, and IT 12,000 to 100,000 µs).

A distortion in the spectrum is observed around 65,000 µs, attributed to saturation of the spectrophotometer. The longer the tube, the longer the integration time. The integration time, which was initially set at 15,000 µs for 10 cm, was optimized to 45,000 µs for 18 cm following a calculation of the signal-to-noise ratio (**Figure 2**).

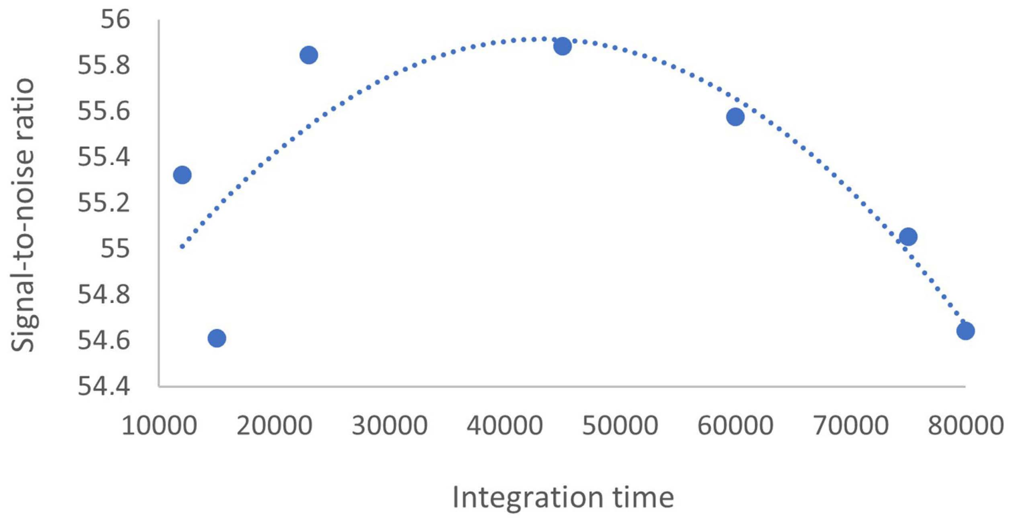


Figure 2. Signal-to-noise ratio of measurements taken with the engine off (seawater pump speed at 600, Scan to Average 30, Boxcar 5, and IT 10,000 to 80,000 µs).

Selecting a few intensity points and calculating the RSB ratio led us to observe an increase up to approximately 40,000 µs, corresponding to an optimal intensity of 45,000 µs.

2) pCO$_2$: The intensity spectra were recorded at a seawater pump speed of 600, with a scan-to-average of 30, a boxcar of 5, and integration times ranging from 15,000 to 45,000 µs (**Figure 3**).

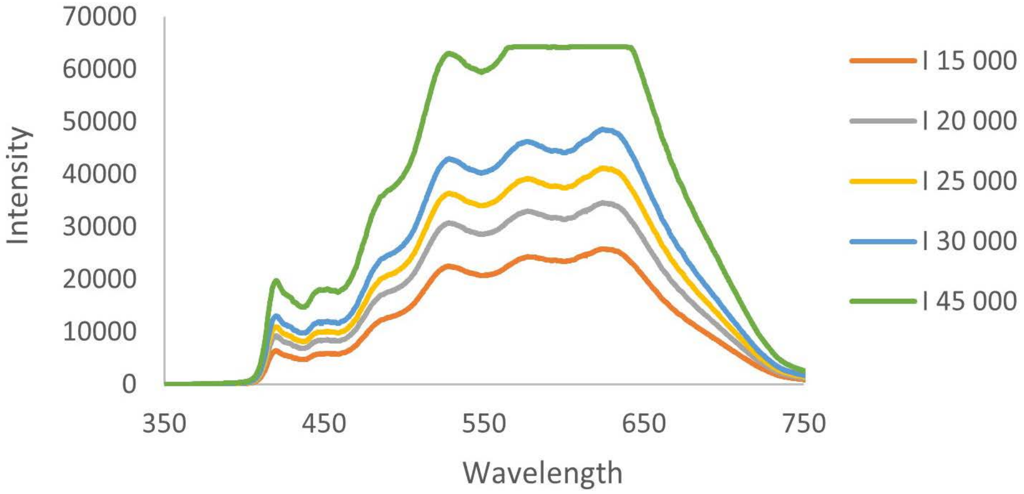


Figure 3. Intensity spectrum measured with the engine off (seawater pump speed at 600 rpm with the engine off; Scan to Average 30, Boxcar 5, and IT 15,000 to 45,000 µs).

A distortion of the spectrum is observed around 60,000 µs, attributed to saturation of the spectrophotometer. The integration time, which was initially set to 350,000 µs for a 10 cm measurement, was optimized to 25,000 µs for an 18 cm measurement following calculation of the signal-to-noise ratio (**Figure 4**).

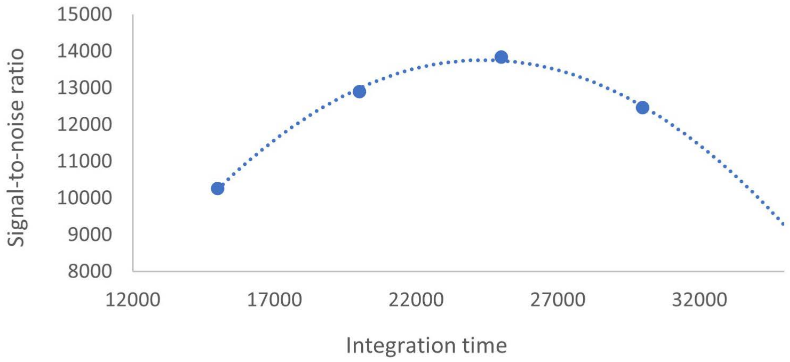


Figure 4. Signal-to-noise ratio spectrum of measurements taken with the engine off (seawater pump speed at 600, Scan to Average 30, Boxcar 5, and IT 12,000 to 35,000 µs).

An increase in noise is observed around 22,000 µs, corresponding to an optimal intensity of 25,000 µs.

2.2. Scan to Average

Scan to Average involves performing several consecutive scans of the same signal, followed by calculating the average of the results obtained. The main objective is to minimize random noise to optimize the accuracy and reliability of the collected data.

Different Scan to Average runs were recorded at speeds of 600 and 50, respectively, for the seawater pump and the dye pump, with an integration time of 22,000 µs and a Boxcar of 0 (**Figure 5**).

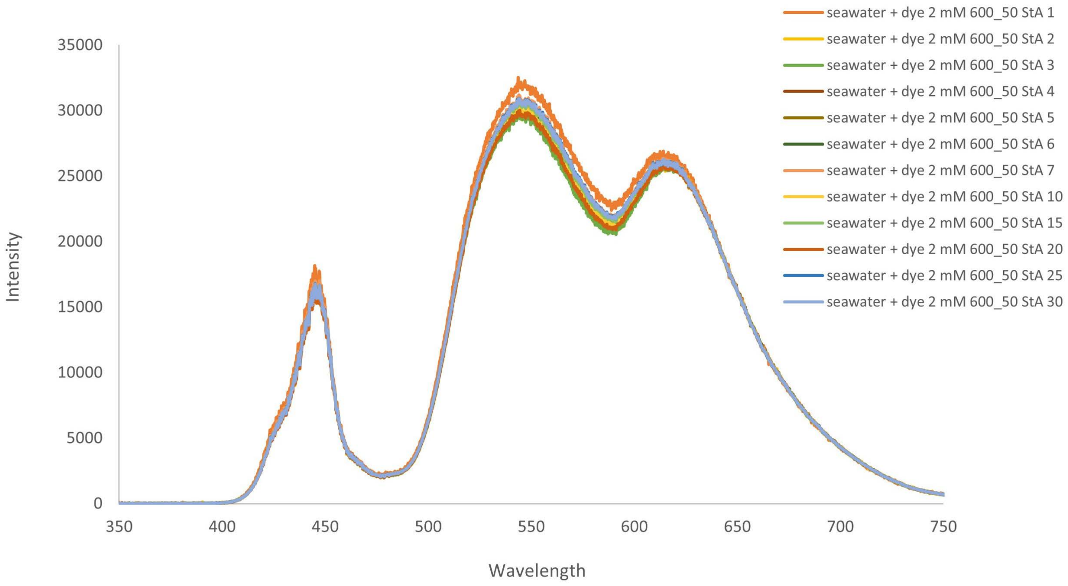


Figure 5. Intensity spectrum of measurements taken with the motors off (pump speed 600 - 50, IT 12,000 µs, Scan to Average 1 to 30, Boxcar 0).

A distortion of the spectrum around 32,000 µs is observed, attributed to saturation of the spectrophotometer, and the RSB ratio was calculated to determine the optimal Scan to Average setting (**Figure 6**).

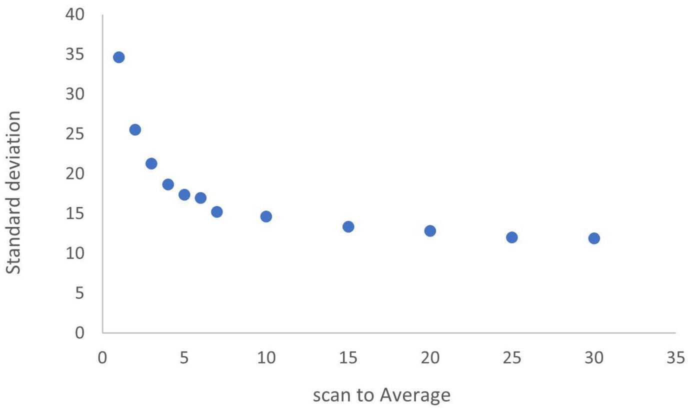


Figure 6. Signal-to-noise ratio spectrum of measurements taken with the engine off (speed 600 - 50, Scan to Average 1 to 30 using 3 replicates and between 675 nm and 750 nm, IT 850 to 1000 µs, and Boxcar 0).

We clearly observe a decrease in the standard deviation as the Scan to Average increases, stabilizing around 15. Subsequently, we chose to work with a Scan to Average of 30.

2.3. Boxcar

The Boxcar filter, which performs digital filtering, uses a uniform average over a data sequence by applying a moving window of constant width. Each filtered data point is determined by calculating the arithmetic mean of the data points within the fixed window centered on that point (**Figure 7**).

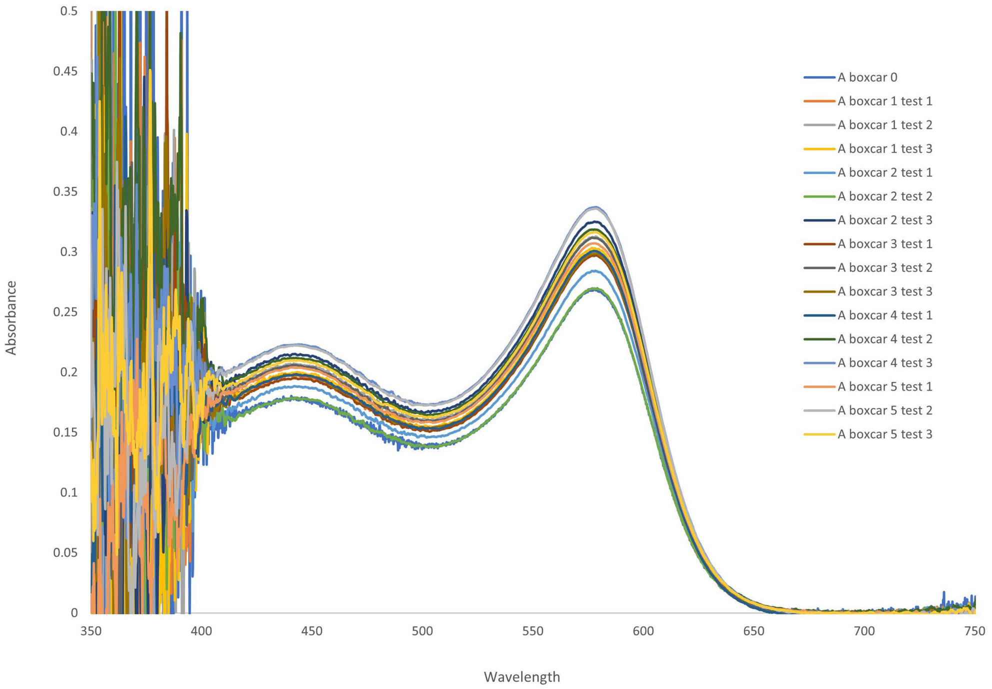


Figure 7. Signal-to-noise ratio spectrum of measurements taken with the engine off (speed 600 - 50, scan-to-average 30, IT 22,000 µs, and Boxcar 0 to 5).

We also measured the standard deviation of the absorbances between 675 nm and 700 nm at different Boxcar values after performing measurements (with engines running) with 3 replicates per Boxcar, except for Boxcar 0, where there were no replicates (**Figure 8**).

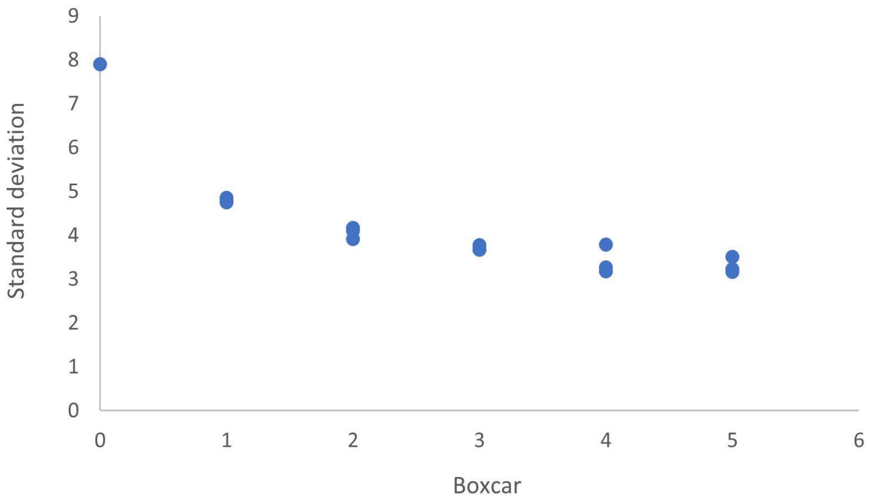


Figure 8. Signal-to-noise ratio spectrum of measurements taken with the engines off (speed 600 - 50, Scan to Average 30, IT 900 µs to 1000 µs, and Boxcar 0 to 5 with 3 repetitions, except at 0, and between 675 nm and 750 nm).

We clearly observe a decrease in the standard deviation as the Boxcar value increases, stabilizing at a Boxcar value of 3. This is why we chose to work with a Boxcar value of 5 thereafter. Furthermore, a Boxcar value of 5 averages over a wavelength range of 1.9 nm on average, which is acceptable.

3. Results and Discussion

Activating a thermostat stabilized the temperature, which had initially been fluctuating, causing the column to rise by 10 to 18 cm. A distortion in the spectral intensity peak indicated detector saturation. The signal-to-noise ratio (SNR) was calculated based on the average of the ratio between the peak of maximum absorbance of the basic form (578 nm for pH and 558 nm for pCO_2) and that of the acidic form (434 nm). The standard deviation of the signal was evaluated in a region where no absorbance is present (between 675 nm and 750 nm).

To refine the measurement parameters, three (3) specific elements were examined: integration time, scan-to-average, and boxcar. The integration time was adjusted (**Figure 2**; **Figure 4**) to optimize the signal-to-noise ratio, a key factor for detecting small fluctuations in pH and pCO_2. The "scan to average" method was used (**Figure 6**) to mitigate instantaneous fluctuations in the data. As for the Boxcar method, it was employed (**Figure 6**) to improve spectral resolution by reducing light interference.

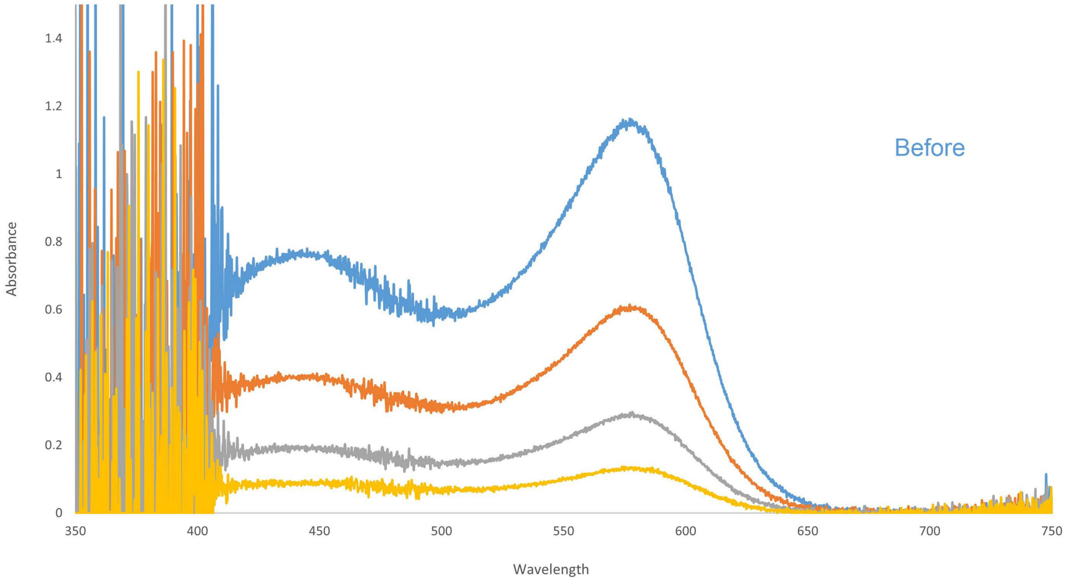
Specific measurement protocols were implemented, including multiple repetitions of each sample to ensure the reproducibility of results. Data collection was automated using Python software (ocapi. v5) to analyze the obtained spectra, ensuring the accuracy and speed of the procedures. These methodological procedures established a systematic and rigorous approach for evaluating spectrophotometer parameters, thereby ensuring reliable results in the study of ocean acidification [8]-[12].

Analysis of the results obtained from optimizing the parameters of the UV-Vis spectrophotometer (OCaPI) reveals key insights into the assessment of ocean acidification in comparison with the results of the experiments conducted prior to optimization (**Figure 9(a)**).

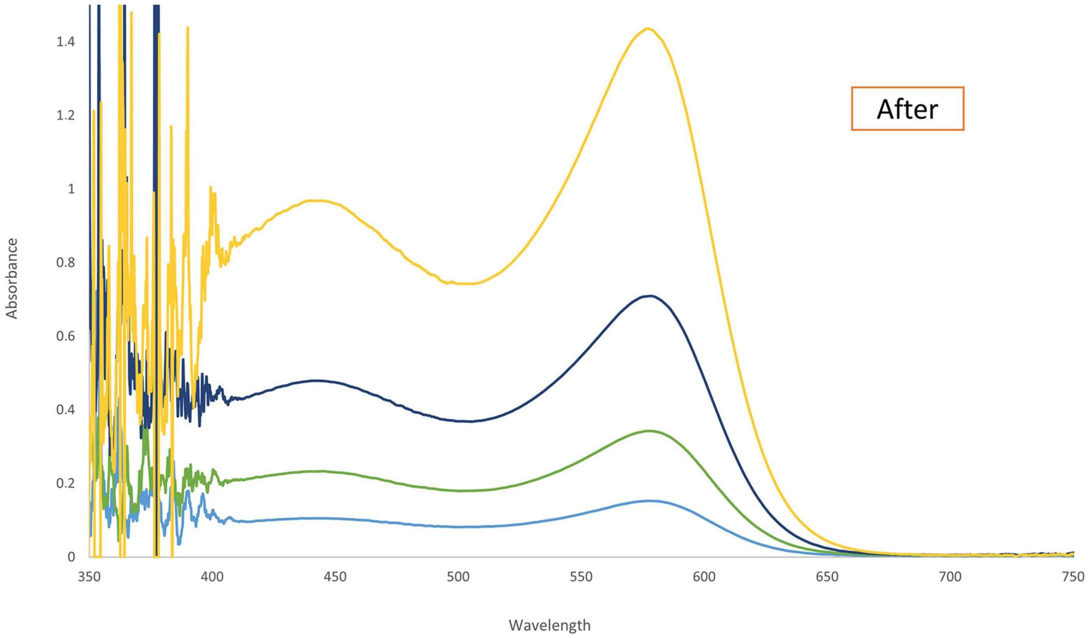
The pH and pCO_2 measurements were examined in relation to variations in integration times, "Scan to Average" settings, and Boxcar parameters. An integration time that is too short can lead to random fluctuations in the data, while a time that is too long could cause drift, thereby altering the results. The selection of the "scan to average" mode is also crucial, as it helps minimize background noise and enhance the signal—requirements essential for detecting the subtle pH variations associated with ocean acidification [2]-[13].

These adjustments (**Figure 9(b)**) led to improved accuracy in detecting low pH levels, which is essential in increasingly acidic marine environments. The collected data revealed a direct relationship between variations in dissolved CO_2 concentrations and pH measurements, thereby confirming the validity of the developed optical method. Furthermore, the results obtained reveal that optimizing integration times to 45,000 µs and 25,000 µs for pH and pCO_2, a scan-to-average of 30, and a boxcar of 5, allows for better differentiation of background noise, thereby providing more accurate measurements, especially in coastal regions where fluctuations are frequent.

However, we opted for a 30-scan "scan to average" method to further reduce random noise and to ensure the 5-point fit was accurate, given its optimal spectral smoothing without significantly broadening the absorption bands.



(a)



(b)

Figure 9. Spectra (a) and (b) show the results before and after optimization, respectively, at pump speeds of 600 - 25, 600 - 50, 600 - 100, and 600 - 200 rpm.

The pH calibration was performed across the full range (certified by the University of California, San Diego), and pCO_2 calibration was performed using certified gases. Each calibration point was tested 10 times in triplicate. Performance was evaluated using a reference CRM solution, which allowed us to achieve accuracies of 0.002 pH units and 2 ppm for the two parameters, respectively.

The optimal parameters mentioned above are specific to the configuration of our tubes and peristaltic pumps, as well as to the Mediterranean Sea (temperature and salinity). A transition to other seawater conditions would require at least a partial revalidation, but the optimization method applies directly.

These observations highlight the need to establish strict protocols for the assessment of these key parameters, with the aim of obtaining measurable and relevant results for monitoring acidification and its effects on marine biodiversity [14] [15].

4. Conclusions

Research on optimizing the parameters of UV-Vis spectrophotometers (OCaPI) to assess ocean acidification has highlighted the vital importance of these analytical instruments for understanding the environmental consequences of climate change.

Given the gradual increase in ocean acidity, it is essential to have precise measurement techniques to monitor pH and pCO_2 levels, as these factors have significant impacts on marine life and ecosystems.

By optimizing the parameters with integration times of 45,000 μs for pH and

25,000 µs for pCO_2, as well as using 30-point "scan to average" techniques and a 5-point Boxcar approach, we were able to demonstrate a significant improvement in the accuracy and reliability of spectrophotometric measurements.

The results obtained not only reveal a correlation with other existing techniques for quantifying these parameters but also offer a new perspective for environmental monitoring by simplifying data collection in challenging environments.

This research therefore paves the way for future applications that could integrate these optimized techniques into long-term monitoring programs, thereby providing valuable insights for the management of marine resources and the preservation of ecosystems in the face of increasing ocean acidity.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

References

[1] Clayton, T.D. and Byrne, R.H. (1993) Spectrophotometric Seawater Ph Measurements: Total Hydrogen Ion Concentration Scale Calibration of M-Cresol Purple and At-Sea Results. *Deep Sea Research Part I: Oceanographic Research Papers*, **40**, 2115-2129. https://doi.org/10.1016/0967-0637(93)90048-8

[2] Wang, Z.A., Liu, X., Byrne, R.H., Wanninkhof, R., Bernstein, R.E., Kaltenbacher, E.A., *et al.* (2007) Simultaneous Spectrophotometric Flow-Through Measurements of pH, Carbon Dioxide Fugacity, and Total Inorganic Carbon in Seawater. *Analytica Chimica Acta*, **596**, 23-36. https://doi.org/10.1016/j.aca.2007.05.048

[3] Zhang, H. and Byrne, R.H. (1996) Spectrophotometric Ph Measurements of Surface Seawater at *In-Situ* Conditions: Absorbance and Protonation Behavior of Thymol Blue. *Marine Chemistry*, **52**, 17-25. https://doi.org/10.1016/0304-4203(95)00076-3

[4] Bégovic, M. (2001) Contribution to the Study of the Carbonate System in the Mediterranean-Spatiotemporal Distribution and Variation of CO_2 Partial Pressure in the Surface Waters of the Ligurian-Provençal Basin. Ph.D. Thesis, Pierre and Marie Curie University-Paris VI. https://theses.hal.science/tel-00002793v1

[5] Louis, J. (2015) Behavior of Biogeochemical Elements in the Mediterranean at the Air-Sea Interface in the Context of Climate Change. Ph.D. Thesis, Pierre and Marie Curie University-Paris VI. https://theses.hal.science/tel-01316537v1

[6] Weiss, R.F. (1974) Carbon Dioxide in Water and Seawater: The Solubility of a Non-Ideal Gas. *Marine Chemistry*, **2**, 203-215. https://doi.org/10.1016/0304-4203(74)90015-2

[7] Wimart-Rousseau, C. (2021) Seasonal and Multi-Year Dynamics of the Carbonate System in Surface Waters of the Mediterranean Sea. https://hal.science/tel-03523187v1

[8] Agilent Technologies (2023) UV-Vis Spectrophotometry. Multiskan SkyHigh Spectrophotomètre pour microplaques.

[9] Agilent Technologies (2019) Cary 60 Catalog. Cary 60 UV-Vis Spectrophotometer Brochure.

[10] Bates, N., Astor, Y., Church, M., Currie, K., Dore, J., Gonaález-Dávila, M., *et al.* (2014) A Time-Series View of Changing Ocean Chemistry Due to Ocean Uptake of Anthropogenic CO_2 and Ocean Acidification. *Oceanography*, **27**, 126-141.

https://doi.org/10.5670/oceanog.2014.16

[11] Davenport, J.J., Hodgkinson, J., Saffell, J.R. and Tatam, R.P. (2015) Noise Analysis for CCD-Based Ultraviolet and Visible Spectrophotometry. *Applied Optics*, **54**, Article 8135. https://doi.org/10.1364/ao.54.008135

[12] Hussain, A.F. (2019) UV-Visible Spectrometry. https://www.researchgate.net/publication/337674152_UV-VISIBLE_SPECTROMETRY

[13] Rérolle, V.M.C., Floquet, C.F.A., Mowlem, M.C., Connelly, D.P., Achterberg, E.P. and Bellerby, R.R.G.J. (2012) Seawater-pH Measurements for Ocean-Acidification Observations. *TrAC Trends in Analytical Chemistry*, **40**, 146-157. https://doi.org/10.1016/j.trac.2012.07.016

[14] Dickson, A.G. and Goyet, C. (1994) Handbook of Methods for the Analysis of the Various Parameters of the Carbon Dioxide System in Seawater. DOE Carbon Dioxyde Survey Science Équipe. https://doi.org/10.2172/10107773

[15] Goyet, C. and Poisson, A. (1989) New Determination of Carbonic Acid Dissociation Constants in Seawater as a Function of Temperature and Salinity. *Deep Sea Research Part A. Oceanographic Research Papers*, **36**, 1635-1654. https://doi.org/10.1016/0198-0149(89)90064-2