ICA2025OSLO
14th IWA Specialised Conference on
Instrumentation, Control and Automation

# A Novel UV-Vis Online Sensor with Modeling Approach for Real-Time Monitoring of Pharmaceuticals in Water

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**Abstract:** This study presents the development and application of a novel UV-Vis sensor with a long optical path length (10 cm) for real-time monitoring of pharmaceuticals in water. The custom-developed sensor demonstrated significantly enhanced detection capabilities, achieving limits of detection (LOD) as low as 3.1 µg/L for tetracycline. While longer optical path lengths generally improve LOD, the rapid attenuation of light intensity over 10 cm of water poses a significant challenge. Our sensor successfully addressed this issue, ensuring accurate and reliable measurements despite the extended path length. The study employed advanced chemometric methods, including data preprocessing (smoothing and derivative transformations) and wavelength selection algorithms (iPLS and CARS), to build accurate predictive models. Remarkably, this advanced model enabled the separate calculation of concentrations for three pharmaceuticals—tetracycline, ofloxacin, and chloramphenicol—even in the presence of significant spectral overlap. The custom sensor's extended optical path length not only improved sensitivity but also facilitated reliable monitoring of these overlapping pharmaceutical mixtures, achieving high predictive accuracy ($R^2 > 0.98$).

**Keywords**: Antibiotics; UV-Vis sensor; online monitoring

The widespread use of pharmaceuticals in households, hospitals, and through pharmaceutical production has led to their accumulation in wastewater, posing significant environmental and public health challenges due to their persistence and potential to disrupt ecosystems[1]. Traditional detection methods, such as gas chromatography-mass spectrometry (GC-MS) and liquid chromatography (LC), offer high sensitivity but are costly, time-consuming, and impractical for real-time monitoring. UV-Vis spectrometry, a faster and more cost-effective alternative, is gaining attention for online pharmaceutical monitoring[2]. However, its limited sensitivity, interference from complex water matrices, and the overlapping spectra of multiple pharmaceuticals hinder its effectiveness. These challenges highlight the critical need for innovative sensor technologies and advanced analytical models that can achieve accurate, real-time monitoring of pharmaceutical pollutants, particularly in high-concentration wastewater from hospitals and pharmaceutical production facilities.

In this research, a novel UV-Vis sensor was developed with two pulsed xenon light sources—one for the reference optical path and the other for the measurement optical path.The sensor has a resolution of 0.5 nm and supports an adjustable optical path length, with a maximum length of 10 cm. The effective detection range spans from 186.5 to 667.5 nm, making it suitable for a wide range of pharmaceutical monitoring applications. The appearance and internal structure of the sensor is shown in **Figure 1.1**, highlighting the key components and arrangement of the light sources, spectrometer, and detectors. **Figure 1.2** displays the spectra for three pharmaceuticals (tetracycline, ofloxacin, and chloramphenicol) measured by both the new sensor and a commercial sensor. The results demonstrate that our sensor provides more stable and sensitive spectral readings compared to the commercial sensor, with clearer peaks and better resolution for overlapping

pharmaceutical mixtures. **Table 1.1** presents the limits of detection (LOD) for the three antibiotics using both sensors. Our custom sensor shows significantly improved LOD values, with detection limits as low as 3.1 µg/L for tetracycline, compared to higher LOD values from the commercial sensor. These results underline the enhanced performance of our sensor, which offers superior sensitivity and accuracy in detecting pharmaceuticals, even in complex water matrices.

This study employed a three-step method to calculate the concentrations of tetracycline, ofloxacin, and chloramphenicol, despite their overlapping spectra. First, raw spectral data were preprocessed using smoothing and derivative transformations to reduce noise and enhance absorption features. Next, wavelength selection algorithms such as interval partial least squares (iPLS) and competitive adaptive reweighted sampling (CARS) identified the most informative wavelengths for each pharmaceutical. Finally, partial least squares (PLS) regression was applied to build predictive models based on the selected wavelengths. As shown in **Table 1.2**, the PLS models achieved high accuracy, with $R^2$ values exceeding 0.98 and RMSEP values as low as 0.846 for tetracycline, 1.888 for ofloxacin, and 3.749 for chloramphenicol. These results represent a significant advancement in real-time pharmaceutical monitoring using UV-Vis spectroscopy.

This research tackles the challenge of monitoring emerging pharmaceutical contaminants in wastewater using a novel UV-Vis sensor and advanced chemometric modeling. The approach enables precise, real-time detection of pharmaceuticals, even in complex mixtures with overlapping spectra, significantly improving the management of hospital and pharmaceutical wastewater. By enhancing sensitivity and accuracy, this study advances water quality monitoring technologies and supports the development of dynamic wastewater treatment systems for better environmental protection.

**Table 1.1** Calculation parameters and limits of detection at different characteristic wavelengths.

| | Mean value of blank sample (1/m) | Standard deviation of blank sample (1/m) | Sensitivity | Limit of detection (mg/L) |
|---|---|---|---|---|
| 280nm (Tetracycline)[a] | 1.26604 | 0.99657 | 3.198 | 0.9349 |
| 290nm (Ofloxacin)[a] | 1.07527 | 1.01339 | 6.542 | 0.4647 |
| 280nm (Chloramphenicol)[a] | 1.26604 | 0.99657 | 2.640 | 1.1325 |
| 273nm (Tetracycline)[b] | -0.00429 | 0.01089 | 10.560 | 0.0031 |
| 286nm (Ofloxacin)[b] | -0.00259 | 0.01052 | 6.990 | 0.0045 |
| 271nm (Chloramphenicol)[b] | -0.00159 | 0.00986 | 0.310 | 0.0954 |

[a] Measure by the commercial sensor
[b] Measure by new developed sensor

**Table 1.2** Performance Metrics of PLS Models for Pharmaceutical Concentration Prediction After Wavelength Selection

| Wavelength selection method | Ofloxacin | | | Tetracycline | | | Chloramphenicol | | |
|---|---|---|---|---|---|---|---|---|---|
| | Ws[a] | RMSEP | $R^2$ | Ws[a] | RMSEP | $R^2$ | Ws[a] | RMSEP | $R^2$ |
| SPA | 5 | 3.30572 | 0.98800 | 5 | 2.45338 | 0.99094 | 3 | 8.51275 | 0.93337 |
| CARS | 16 | 2.49126 | 0.99281 | 6 | 0.84635 | 0.99873 | 13 | 3.74908 | 0.98767 |
| iPLS | 9 | 1.88800 | 0.99528 | 9 | 1.75843 | 0.99600 | 28 | 4.13771 | 0.98305 |

[a] Number of wavelengths selected

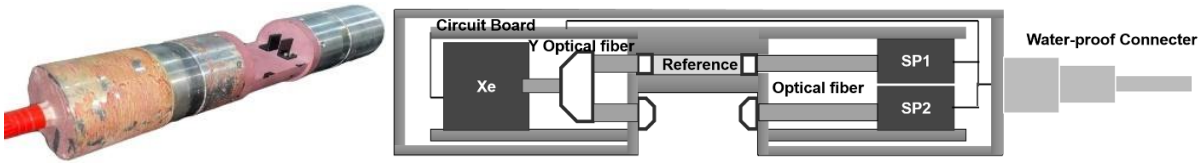


**Figure 1.1** The appearance and internal structure of the new UV-Vis sensor

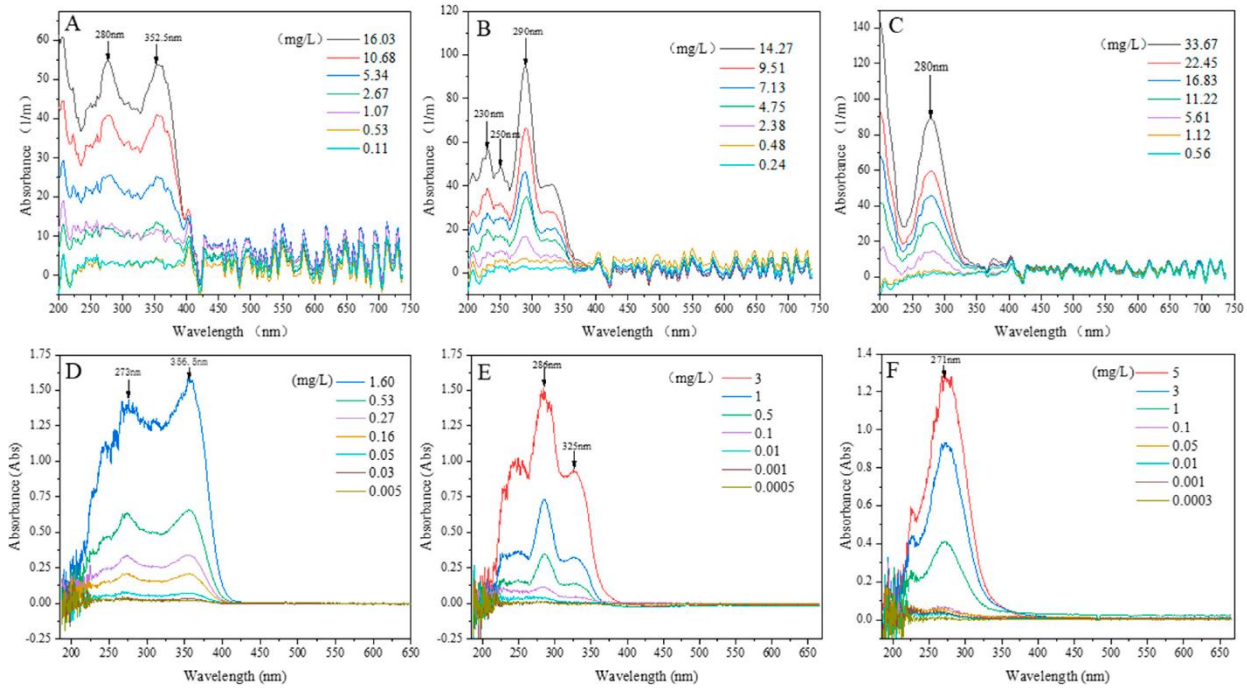


**Figure 1.2** Absorption spectra of (A) tetracycline, (B) ofloxacin, and (C) chloramphenicol by a commercial sensor and (D) tetracycline, (E) ofloxacin, and (F) chloramphenicol by new developed sensor

## REFERENCES

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