

Information systems for assessing the environmental impact of industrial processes

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Outline

1. Introduction
2. Related Work
3. Project overview
4. Conclusion

Analytical parameters

- Chemical Oxygen Demand (COD)
- Biochemical Oxygen Demand (BOD)
- pH, conductivity, hardness...

Analytical parameters

- **Chemical Oxygen Demand (COD)**
- Biochemical Oxygen Demand (BOD)
- pH, conductivity, hardness...

Objectives

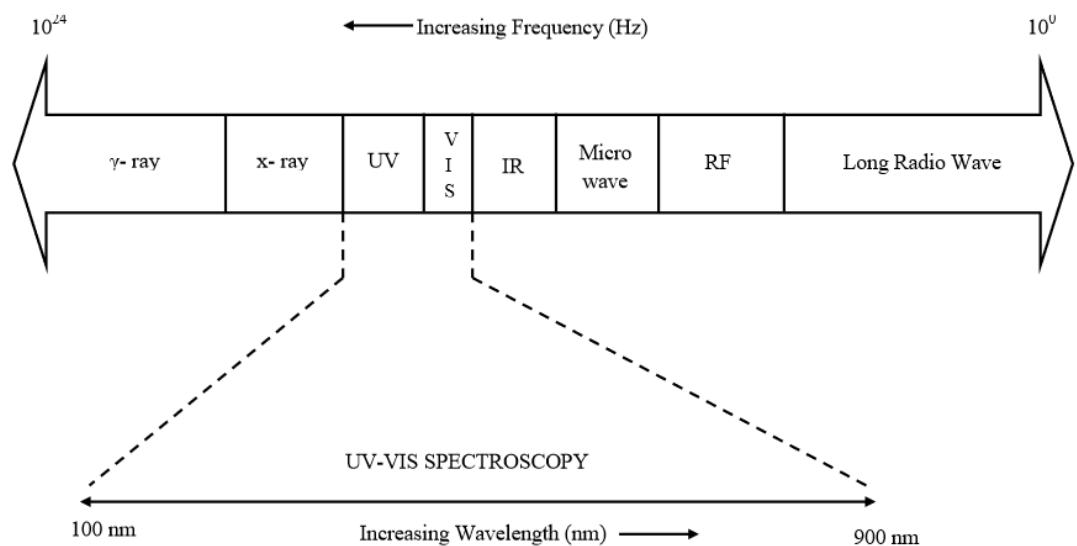
- Build a continuous **monitoring system**
- Reduce laboratory **analysis cost**
- Limit air and water **pollution**

Current method

- Titrimetric analysis
 - Laboratory
- Chemometrics
 - Data-driven

Spectrum

- Ultra-violet and Visible (UV-Vis) spectroscopy

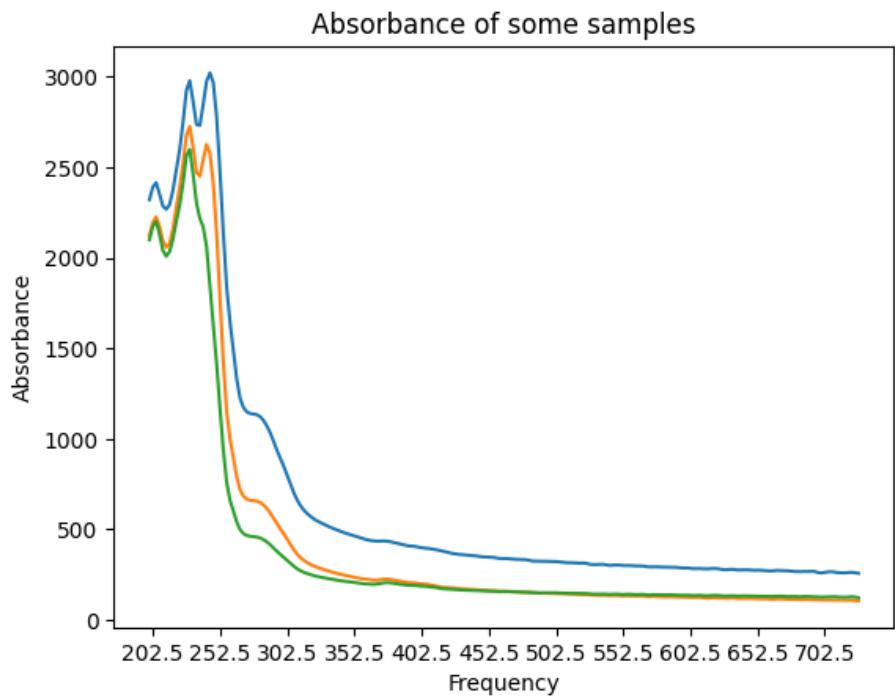


Spectrum

- Ultra-violet and Visible (UV-Vis) spectroscopy
- Beer-Lambert law

Spectrometer

- Absorbance
- Limitations:
 - Optical sensor



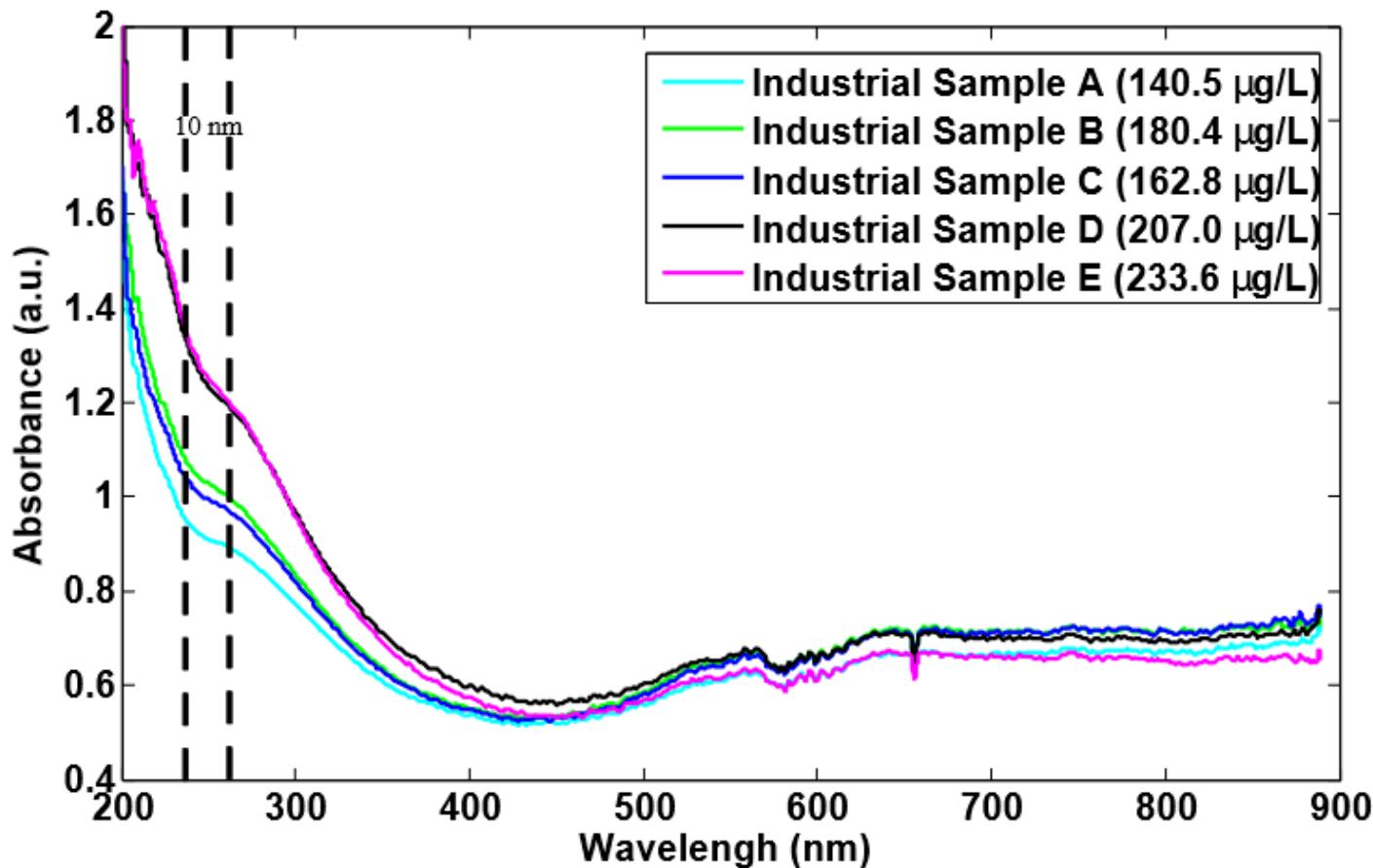
Related work

Collect absonbance

Select a wavelenght

Build linear regressor

Related work



Related work - drawbacks

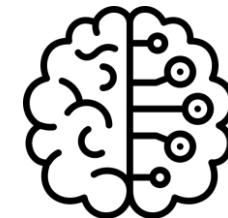
Laboratory prepared samples

One wavelength

Linear regressor stiffness

Our project

- Machine Learning
- Life Cycle Assessment



Project overview



Predict the level of pollutants in
wastewaters



Monitor the pollutants

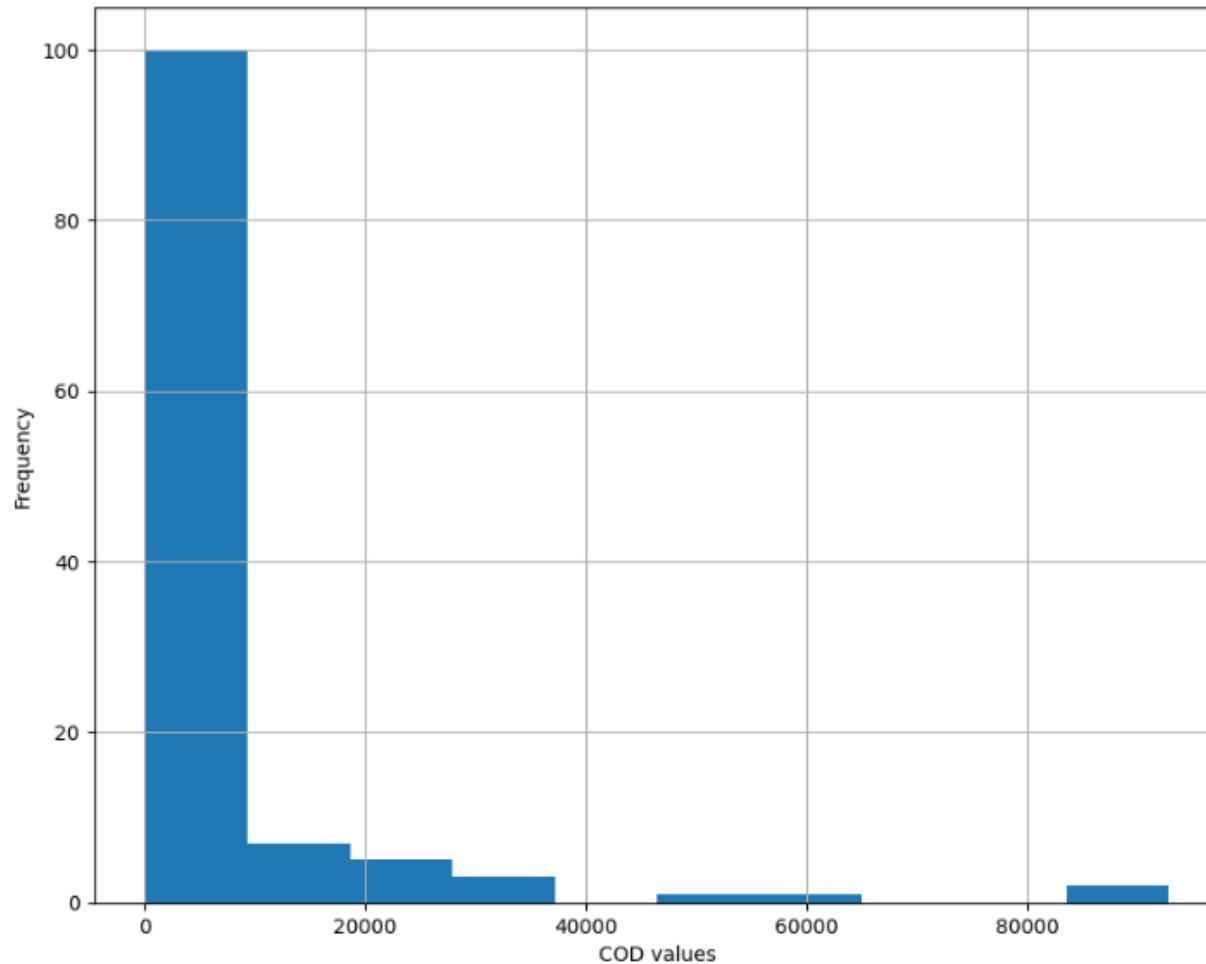


Simulate the production varying chemical
agent

Dataset

- 212 features
- 119 samples

Data distribution



Estimating COD

- Principal Component Analysis (PCA)
- Compare Machine Learning Algorithm

Evaluation measures

- RMSE

$$RMSE = \sqrt{\sum_{i=1}^n \frac{(\hat{y}_i - y_i)^2}{n}}$$

- R²

$$R^2(y, \hat{y}) = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2}$$

Results

Model	RMSE		R2	
	Training	Validation	Training	Validation
Null model	14484.14	14165.42	0.00	-0.25
Ridge Regression	275.16	36052.17	0.99	-7.30
Random Forest	4164.05	10638.99	0.86	0.29
SVM	2661.48	4329.57	0.95	0.77
MLP	3522.22	6548.99	0.92	0.55
KNN	7845.81	10672.14	0.68	0.30

Conclusion and next steps

- Objective: Construct a reliable system to constantly monitor pollutants
- Analyse how our work may impact on industries
- Does a chemical agent impact on the pollution?

Thank you!

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