Section Sciences et Ingénierie de l'environnement
Design Project 2023 (semestre de printemps)

Proposition n°12

Development of tools to understand air pollution measurements from novel instrumentation

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Partenaire externe ou laboratoire IIE

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AeroSpec (incubating at LAPI, EPFL, under the Innogrant)

Taille de l'entreprise (nbre de collaborateurs) : Incubating startup (2 members)

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Site Web www.aerospec.ch (under construction)

Encadrant EPFL

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Descriptif du projet

The project involves extending and developing codes on analysis of infrared spectra for atmospheric aerosol composition analysis. There is already a large source of codes that have been developed for IR analysis on Polytetrafluoroethylene (PTFE) filters, and this project will develop new codes for certain analysis aspects and adapt the existing analysis codes to measurements using a new instrument that does not use the filters. Apart from coding, use of statistical methods is needed to make proper analysis.

Infrared spectroscopy of particulate matter (PM) has garnered special attention in recent years for providing numerous atmospheric indicators with a single analytical technique [S. Takahama et al. doi: 10.5194/amt-12-525-2019] that has otherwise been challenging using conventional methods. It is unique as it not only measures a vast majority of chemical information of PM in the form of functional groups (FG) concentrations of organic mass, inorganic salts and mineral dust, but also leverages the information for reconstructing total PM mass, OM:OC ratio, EC and metal concentrations [B. Debus et al. doi: 10.5194/amt-15-2685-2022, A. Yazdani et al. doi: 10.5194/amt-2020-79].

Recently, a new instrument has been developed at the startup "AeroSpec", where they aim to make chemical composition analysis of aerosol more widespread and adaptable, to allow

better particulate matter analysis and policy making. To do this, the infrared aerosol monitor (IR-AM) instrument has been developed as an automated aerosol collector (for PM$_{2.5}$) that performs IR spectroscopy on the particles and then self-cleans itself. The final aspects of automations are currently underway. The new IR spectra from this IR-AM instruments will require its own codes to function properly.

The project involves:
- Understanding IR spectroscopy basics and concept and inherent meaning of peak intensities, baselines, peak shifts, peak fitting, scattering and other optical effects (we can guide you for swift learning)
- Reading and understanding the current code base (for measurements on PTFE filters), written in R language
- Coding wrappers in Python for these R packages of IR-analysis to make it compatible with IR-AM instrument measurements
- Experimenting with new codes on certain analysis aspects – for example, advanced baseline correction, or concentration retrieval.
- Evaluating the performance of the codes on a large number of spectra to analyze statistical biases, correlations and overall performance
- Discussing and explaining the code performance for the IR measurements and providing suggestions for the future work
- Guidance and assistance will be provided at every step.

Objectif et buts

Objective:
Verify and evaluate the current IR analysis codes on a new IR measurement method using a novel IR-AM instrument; and subsequently developing new codes based on scientific understanding of infrared spectroscopy.

Realistic goals:
- Evaluation of existing IR analysis codes on those from the new IR-AM instrument
- New python codes for analyzing the IR spectra
- Write a report on the findings, compiling the response of the IR analysis results to the various codes and scientifically analyzing the results.

Descriptif tâches

- Scientific: Reading and learning literature on 1) IR-spectroscopy (especially for organic molecules) and 2) IR analysis of PM.
- Computer coding and statistics: Understanding the current IR analysis of PM codes that have been written on R language
- Computer coding and statistics: Writing new codes and adapting the existing ones to evaluate the IR spectra as obtained from the novel IR-AM instrument
- Scientific: Analyzing the accuracy and precision of the different code analysis methods and arguments on suggesting the preferred method and making recommendations for the future.

Divers

A number of skills have been listed in the different tasks – as all the skills are quite diverse, we are happy to train the students on their desired skills and guide the project at every step.