Rui Filipe Cantarino Valente de Almeida

Master of Science

Development of a Tomographic Atmospheric Monitoring System based on Differential Optical Absorption Spectroscopy

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of the requirements for the degree of

Doctor of Philosophy in
Biomedical Engineering

Adviser: Pedro Vieira, Auxiliar Professor,
NOVA University of Lisbon

FACULDADE DE
CIÊNCIAS E TECNOLOGIA
UNIVERSIDADE NOVA DE LISBOA

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Glossary

aliquam	tincidunt urna. Nulla ullamcorper vestibulum turpis. Pellentesque cursus luctus mauris.
computer	An electronic device which is capable of receiving information (data) in a particular form and of performing a sequence of operations in accordance with a predetermined but variable set of procedural instructions (program) to produce a result in the form of information or signals.
cras viverra	metus rhoncus sem. Nulla et lectus vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat.
donec nonummy	pellentesque ante. Phasellus adipiscing semper elit. Proin fermentum massa ac quam. Sed diam turpis, molestie vitae, placerat a, molestie nec, leo.
integer sapien	est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem vel leo ultrices bibendum. Aenean faucibus.
lorem ipsum	dolor sit amet, consectetuer adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris.
maecenas lacinia	nam ipsum ligula, eleifend at, accumsan nec, suscipit a, ipsum. Morbi blandit ligula feugiat magna. Nunc eleifend consequat lorem.
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nam lacus	libero, pretium at, lobortis vitae, ultricies et, tellus. Donec aliquet, tortor sed accumsan bibendum, erat ligula aliquet magna, vitae ornare odio metus a mi.
nam dui	ligula, fringilla a, euismod sodales, sollicitudin vel, wisi. Morbi auctor lorem non justo.
name arcu	libero, nonummy eget, consectetuer id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo.
nulla malesuada	porttitor diam. Donec felis erat, congue non, volutpat at, tincidunt tristique, libero. Vivamus viverra fermentum felis.
sed lacinia	nulla vitae enim. Pellentesque tincidunt purus vel magna. Integer non enim. Praesent euismod nunc eu purus. Donec bibendum quam in tellus.

Acronyms

AP	Air Pollution
DOAS	Differential Optical Absorption Spectroscopy
EPA	Environmental Protection Agency (United States)
FFF	Forest Fire Finder
ML	Machine Learning
PM	Particulate Matter
RQ	Research Question
WHO	World Health Organization

Symbols

*

Chapter 1

Introduction

1.1 Background and Motivation

1.1.1 Background

The idea behind this thesis was born in 2015, at NGNS-IS (a Portuguese tech startup). At the time, the company's flagship product was the Forest Fire Finder (FFF), which was a forest fire detection system that performed a spectroscopical analysis of the atmosphere and then, through some Machine Learning (ML) techniques, could detect the presence of a smoke column above the horizon and alert the operators.

The growing importance of Air Pollution (AP) in today's society, and the fact that the system was already scanning the atmosphere for some chemical components originated and motivated the idea behind this thesis. Although FFF was already a spectroscopic system, it was constructed to operate in remote and inhospitable locations, and its design had had no spatial constraints into account. In addition, the system scanning method (depicted in Figure **??**) meant that it was not appropriate for pollution measurement, as it could only detect a mean pollutant column density for each spectrum it took. A truly useful monitoring tool would be able to map these pollutants concentration, thus retrieving the same kind of information as a network of in-situ electro-chemical sensors.

This ambition also brought novelty to the project, since to the best of the team's knowledge, a similar system had not yet been developed, a situation that has remained the same up to the current days.

1.1.2 The Problem

Air Pollution (AP) is one of the grave concerns of modern day western society, with many decades worth of research proving that it can have a pronounced negative effect on human, animal and plant life, as shown in Section **??**. On humans, it has been shown to significantly increase risk of cardiovascular, pulmonary and even neuropsychiatric diseases [1–3]. Its implications on ecosystems are remarkably complex and difficult to quantify, but nonetheless extremely important, and have a huge impact on biodiversity [4].

Knowing all this brings us the responsibility of at least trying to mitigate some of these adverse consequences of the spectacular progress that we have achieved in the few last centuries. But we cannot act unless we also know what we must do; and to know this, we must have measurements.

1.1.3 Objectives

The overarching goal of this thesis was to theorize and design a bidimensional mapping tool for trace atmospheric pollutants such as NO_x and SO_x, using Differential Optical Absorption Spectroscopy (DOAS) as the measurement technique. During the research, several "micro-objectives" appeared regularly. Some were kept and incorporated in the workplan, others discarded after initial exploration. The main secondary objectives, which had a very heavy influence over the adopted methods, were:

- To use a tomographic approach for the mapping procedure;
- To use a single collection point, minimizing material costs for the technology.

1.1.4 Methods

To answer this question, I

1.1.5 Results

1.1.6 Conclusions

Chapter 2

Research Question

2.1 Problem Introduction

AP is a very important topic of discussion in the current days, with scientists and researchers around the globe being very well aware of the potential effects it can have on the health of individuals and populations across all ecosystems. Not to mention its implications on climate change, which are generally regarded as one of the capital threats to life on Earth's survival (on par with a nuclear apocalypse). Defining AP can be a challenge. In fact, its effects and presence is so all-encompassing, that it would be fair to say that its definition changes with the angle with which one looks upon it. Nonetheless, it is important to at least try to define it, in order to approach it in some way [2, 4].

The United States Environmental Protection Agency (EPA) defined Air Pollution (AP) as "*the presence of contaminants or pollutant substances in the air that interfere with human health or welfare, or produce other harmful environmental effects*" [5]. This is (perhaps intentionally) a very broad definition, too broad to avoid vagueness. It does introduce a key concept: the term *pollutant*, which needs be discussed in order to complete the definition above.

It would be very hard to find someone who did not have an almost instinctive idea of what a pollutant is. We know something is amiss when we notice our air is full of smoke or smells strange, but our senses are not enough. There are many chemical components that are untraceable by unaided humans, and some that are only detected by our noses and eyes at concentration levels which are above the threshold where they can damage our health. This makes the task of separating pollutants from non-pollutants a non-trivial one. If we cannot rely solely on our senses to detect them, then it is up to the scientists and engineers to create methods that allow us to do so. Whats more, we must also rely on them to understand how can a normally harmless substance be a pollutant, depending on the circumstance. For instance, nitrous compounds are traditionally beneficial to the soils and cultures, but they can and do cause pulmonary and cardiovascular complications in humans [1–3].

Context matters to pollutants. The toxic nature of a certain chemical only is revealed when someone or something gets exposed to it. Even then, there are exposure levels which do not bear any effects, good or bad. At these levels, a pollutant is but an impurity. There too many potential pollutants in our modern day world to list here, but the World Health Organization (WHO) states that there are six major air pollutants:

- Particle Matter (PM);
- Ground level ozone (O_3);
- Carbon monoxide (CO);
- Sulfur Oxides (SO_x);
- Nitrous Oxides (NO_x);
- Lead (Pb).

Exposure to these pollutants have different effects on humans, ranging in seriousness from skin irritation to neuropsychiatric complications, depending on dose and on the time the exposure lasts.

2.2 Research Question

In Chapter 1, I have introduced the reasons which led NGNS-IS to pursue the development of an atmospheric monitoring system, and that what set it apart from other systems was the ability to spectroscopically map pollutants concentrations using tomographic methods, thus defining a primary objective for this thesis.

Two secondary objectives were born from the necessary initial research, which had a very heavy influence over the adopted methods:

- To use a tomographic approach for the mapping procedure;
- To use a single light collection point, minimizing material costs.

Taking all the above into account, we arrive at the main Research Question (RQ), presented in Table **??**.

Table 21: Main research question.

RQ1	*How to design a tomographic atmosphere monitoring system based on DOAS?*

This is the main research question. It gave rise to four other more detailed research questions. These secondary questions allow a better delimitation of the work at hand and are important complements to RQ1. This questions are presented in Table **??**

Table 22: Secondary research questions.

RQ1.1	*What would be the best strategy for the system to cover a small geographic region in an urban setting*
RQ1.2	*What would be the necessary components for such a system?*
RQ1.3	*How will the system acquire the data?*
RQ1.4	*What should the tomographic reconstruction look like and how to perform it?*

2.3 Hypothesis and Approach

This work is based on the hypothesis that a system such as the one described in Chapter 1, which responds to the RQ in Table **??** and Table **??** can be achieved by careful selection of mathematical tomographic algorithms and instrumentation that is able to implement them correctly.

Pursuing this hypothesis will naturally lead to answering all the research questions, both primary and secondary. This will involve studying the literature in at least two fronts: on one hand, I will have to search and implement the tomographic part of the project; on the other, I will have to study and select the main system components. Both tasks seem reasonably independent, but in truth they are not. Whatever the components will be, they will have to be capable of implementing the algorithms, and conversely, the algorithms should be chosen in such a way that it does not make the instrumentation too costly or impossible to assemble.

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Chapter 3

Literature Review

Chapter 4

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