Tomographic DOAS - a Systematic Mapping Study on its technological status

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Abstract

In atmospheric chemistry and physics, DOAS is one of the most commonly used analytical techniques. The method allows the application of tomographic reconstruction procedures for 2D or 3D mapping of target trace gases' concentrations.

Tomographic DOAS applications have been documented for at least 20 years. The number of articles detailing its implementation, however, is low, and literature is sparse. This paper aims to catalogue publications on this subject, painting a quick picture of the field's technological landscape.

Our search has found that there is a great prevalence of active DOAS systems in Tomographic DOAS research activities, since we were unable to find a passive application. We can also infer that there is no current commercial application using this technology and while it is true that there are similarities between different groups' apparatus, there is still no uniform application.

Our initial search has rendered more than 700 articles. However, the application of our inclusion and exclusion criteria resulted in a final set of 8 papers detailing the tomographic equipment, reconstruction algorithm and software. From them, we were able to identify some common practices and possible research gaps.

Keywords: DOAS, Tomography, Systematic Mapping Study

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1. Introduction

Differential Optical Absorption Spectroscopy (DOAS) is one of the most prominent methods for analysing and quantifying atmospheric chemistry, namely in what concerns trace gas concentrations. The technique, developed during the 70s by Perner and Platt [20], was popularised in the following decades by its use in detecting Ozone, Nitrogen Oxydes and studies of cloud radiative transport. DOAS is a type of absorption spectroscopy, which uses a clever mathematical and physical observation to overcome the difficulties of spectral measurement in the open atmosphere.

Through the setting of very careful geometric considerations, it is possible to combine DOAS with tomographic reconstruction methods in order to assemble a map of the gaseous concentrations in a given geographic region. Tomography is the process of reconstructing an image through projections obtained by subjecting a given target (in our case, the atmosphere) to being traversed by any kind of penetrating or reflecting wave, which in our case is visible light.

With this study, we have intended to capture the current literary landscape surrounding the usage of tomographic DOAS, assessing this technique's technological status. For this purpose, we have employed a review methodology originary from Evidence Based Medicine. This method, which has migrated to engineering through Software Engineering, is called a Systematic Mapping Study (MS). It provides a framework that allows researchers to produce detailed and systematic search protocols, which are used to catalogue literature information and identify research gaps within a determined subject.

The search procedure that we have defined was carefully engineered to cover all tomographic DOAS research relevant to urban, rural or industrial environments. Through it, we were able to find several different applications, all pertaining to scientific research, which are similar regarding physical principle, but differ in equipment assembly, algorithms, software, and geometry.

The rest of this paper has the following structure: Section 2 presents the context within which this study was written; Section 3 describes how we have planned to perform the study and the methods we have used in doing it; Section 4 describes the application of the said methods in the pursuit of our goals and presents the results we have obtained, as well as our evaluation of our processes; Section 5 shows our conclusions and what we think might be retained from reading this paper.

2. Background

2.1. Differential Optical Absorption Spectroscopy

Absorption Spectroscopy is the term used to identify all techniques that use radiation absorption by matter to assess and quantify elements or molecules in a given spectroscopic sample. It had, and still has, a very important role in the study of the Earth's atmosphere [22].

It is, as many other spectroscopic techniques, based on Lambert-Beer's law, which states that 'in a medium of uniform transparency the light remaining in a collimated beam is an exponential function of the length of the path in the medium', as described originally by Pierre Bouguer in 1729, and can be written [22]:

$$I(\lambda) = I_0(\lambda) \cdot \exp[-L \cdot \sigma(\lambda) \cdot c] \tag{1}$$

In Equation 1, I is the light intensity as measured by the spectrometer, I_0 the original light intensity at the source, L is the optical path in which the sample is exposed to the light, σ is the optical cross section of the sampled element or molecule and c is the sample's concentration. λ is the radiation's wavelength.

Lambert–Beer's equation, while valid in a laboratory setting, is generally not enough to determine gaseous concentrations in an open atmosphere experiment. I_0 determination would require require any absorbant from the medium, which is impossible. Besides, in this medium, there are many factors that influence measurements: Rayleigh's scattering, Mie's scattering, thermal variations, turbulence and instrumental transmissivities. All these play an important part in altering atmospheric light [22, 16].

Differential Optical Absorption Spectroscopy (DOAS) overcomes these difficulties by capitalising on cross section's differences between interfering phenomena (normally broad spectral features) and certain trace gases (usually narrow spectral structure). The mathematical formulations behind the technique are well beyond the scope of this article, but suffice it to say that the broad structures are removed through subtraction of a fitted low order polynomial, and a fitting algorithm (such as Levenberg-Marquardt) is used to retrieve concentrations. Detailed presentations of these procedures are presented in [22] and [16].

In [22], the authors split the DOAS method into two fundamental families: passive and active. The passive family is characterised by being designed to capture and analyse natural light, whether from the Sun, the Moon or any other celestial body. This kind of measurement has the advantage of being simple to assemble, but natural light usage implies an additional technical effort for the retrieval of atmospheric concentrations. Active DOAS applications, on the other hand, use artificial light sources to make their measurements. This has been used extensively in the identification of several atmospheric components. Its concentration extraction procedure is simpler, at the expense of a more complex assembly.

DOAS has had a number of applications throughout the years. The technique was first applied in the 1970s. At that time, Perner used an active setup with a laser light source to identify the OH radical in the atmosphere [20]. More recently, researchers around the world have been employing broadband sources (such as Xenon lamps) to measure trace gases like Ozone, Nitrogen Dioxide or Sulphur Dioxide. Almost simultaneously, passive systems have been used to study stratospheric chemistry and radiative transport in clouds [22].

2.2. Multi-Axis DOAS

Multi-Axis DOAS (MAX-DOAS) is one of the more recent applications of the DOAS technique. It represents a significant progress regarding zenith scattered sunlight measurements, a well established atmospheric analysis technique. It performs a series of passive DOAS measurements in several telescope elevations (typically 4 to 10) [11], either in sequence or simultaneously.

MAX-DOAS stems from another set of techniques called *off-axis*, which in this case means that the telescope is pointed at another angle than the zenith. Off-axis DOAS was first employed in 1993 when Sanders et al. [25] used it to assess OClO in Antarctica. During this experiment, the team concluded that the off-axis geometry greatly improves sensitivity for tropospheric species, but does not change the system's ability to quantify stratospheric absorbers.

By evaluating several directions, the technique allows researchers to measure not only stratospheric contributors, as zenith sky assemblies, but also to detect absorbers at ground level, as an active DOAS instrument would.

We mention MAX-DOAS in this paper because one could argue that these systems would be able to be adapted to perform tomographic measurements, if more than one system would analyse the same region from more the same number of observation angles. MAX-DOAS tomography is a special case, and would probably deserve to be investigated fully. However, since this was not the object of our study, we chose not to specifically target this method in our search.

2.3. Imaging DOAS

Imaging DOAS combines spectral and spatial information by combining an imaging spectrometer with a scanning system. The resulting data clearly resembles that of a hyperspectrum **??**.

The method, developed by Bobrowsky et al. [2], employs a 2D CCD detector. One dimension measures spectral information, while the other contains spatial information for one direction. The other spatial direction is obtained by scanning the field of view with the pushbroom method.

DOAS is used to yield slant column density values for the absorbers for each pixel. The values are colour coded and produce an image describing the gas distribution.

Mention to this technique is included in this paper because it exists in order to produce a two-dimensional image from spectral information. This image, however, does not come from a tomographic reconstruction procedure, nor is spatial information recovered from projections, but instead comes directly from the acquisition method. Hence, we did not include articles on this method in this study.

2.4. Tomography

Tomography refers to the set of techniques that aim to produce a cross sectioning image from data collected by exposing a given target body to some kind of penetrating or reflecting wave from many different directions [9, 13].

The initial theories that gave rise to tomography were laid out by Johannes Radon in 1917, with a mathematical operation that would later be known as the Radon transform. This process maps a function f, defined in the plane, to the function Rf, comprised of the values of the line integrals of f, taken in θ directions. In practice, this formulation allows the reconstruction of an image by its projections, which are nothing more than line integrals [4].

Tomographic image reconstruction can be achieved by running one of several algorithms through a computer program. The presentation of these algorithms is completely beyond the scope of this article, but a good starting point for learning about these operations is *The Mathematics of Medical Imaging*, by Timothy Feeman [4]. It is in the scope of this article, however, to make a small introduction to a particular set of reconstruction methods. The reason for this being the prevalence of these methods in the field of DOAS tomography, which is the main subject of this study. These techniques are thus:

Algebric Reconstruction Techniques (ART) Proposed in 1970 by Gordon and Herman [10], these techniques are based on successive approximations between the actual projection data and the sum of the reconstruction elements which represent it [5]. The process is conducted line by line, until a satisfactory convergence condition is met.

Simultaneous ART Simultaneous ART is very similar to the ART algorithm. The difference being that the iterative changes occur for all lines at the same time, instead of in only one.

Simultaneous Iterative Reconstruction Techniques (SIRT) The main difference between SIRT and SART is that in the former, cell changes are not reflected immediately after one calculation. Updates occur at the end of each iteration. At this point, the change for each cell is the average correction calculated for it taking all equations into account [12].

During the second half of the twentieth century, tomographic processes have had a revolutionary influence in many fields of study, but especially in medicine. Computational tomography scanners allow doctors to see their patients interior in a highly detailed and extremely safe fashion. At first, tomographic imaging was performed only with X-Rays. Their attenuation throughout the patient's body being used as a projection. Nowadays, there are much more methods of image retrieval, such as radioisotopes, ultrasound or particle anihilation [13, 4, 9].

Although it was the field of medicine was more influenced by tomographic procedures than any other, the applications of these methods are not restricted to it. One can find numerous industrial and research applications [1, 6, 3]. One of which is the application to atmospheric research, namely in conjunction with DOAS. In recent years, scientists have been working on tomographic methods for measuring atmospheric trace gas concentration values. The field is interesting because it allows for 2D or even 3D mapping of a given region, with respect to those trace gases. This article aims to make an assessment of the status of this tomographic application, by analysing current literature on the subject.

2.5. Mapping Study

A Systematic Mapping Study (MS) is a type of secondary study designed to determine the general features of the research landscape in the subject they are addressing [14, 21].

An MS is driven by broad (and often multiple) research questions and applies an also broad data extraction protocol. This is in line with the fact that this kind of study aims to summarise its findings, answering the research questions, and in-depth analysis is not required. It is common for an MS to be a precursor to a Systematic Literature Review (SLR), which is a much deeper kind of systematic study. Guidelines for performing studies of both kinds can be found in a report made by Kitchenham and Charters in 2007 [14]. In this document, the authors establish the 3 stages which all MS and SLR generally have:

Planning This stage includes all preliminary considerations regading the MS or SLR in the making. All protocols, from search to evaluation, through data extraction, are devised;

Conduction During this staged, researchers apply what they have planned in the previous phase. Protocols are *actually* run, and data is synthesised;

Reporting In this phase, the team has to define their dissemination strategy, and implement it. It is in this stage that a final report is written and evaluated.

Although it is logical (and fundamentally correct) to assume that these steps are sequential, this may not be, and usually is not, accurate. Many of these stages and their intermediate steps require iteration. For instance, some inclusion or exclusion criteria may only be found necessary once the search protocol is implemented.

3. Methods

In the elaboration of this article, we took the three normal stages of SLR conduction: planning, conduction and reporting. The first stage involves making the decisions that guide the rest of the process; the conduction phase is comprised of the actual gathering of data, using the protocol defined in the first stage. The final section of the study is basically the writing and the publishing of the results. In this section, we present the methods used in the study and their rationale, which roughly corresponds to the planning stage.

3.1. Objectives

An MS always aims to answer its research questions in a broad but definite way. It is a way of understanding a given field of research, and being able to systematise how this understanding is achieved.

As stated before, this is an MS aimed at characterising DOAS tomography general status. In doing this, we pretend to get a clearer image of what has been done and what should be attempted next, hopefully managing a sort of roadmap for future research contributions.

3.2. Research Questions

We have begun by defining the goals for our study, and structuring them with a PICOC (Population, Intervention, Context, Outcome and Comparison) analysis, which is summarised in Table 1. This analysis led us to our research goal: *to assess the technological status of the DOAS tomography technique*.

We used this goal statement as a primer to our research question, which was then formulated as: **what is the current status of the technology used in tomographic DOAS?**

Table 1: *PICOC analysis.*

Population	DOAS research in general.
Intervention	The papers must address tomographic DOAS.
Outcome	Status **assessment** for **DOAS tomography**.
Context	Research papers.

Table 2: *Research question slicing*

Original	What is the current status of the technology used in tomographic DOAS?
RQ1	Is there a typical hardware setup used in tomographic DOAS studies?
RQ2	Is there a standard software used to perform these analysis?
RQ3	What are the algorithms more commonly used?

Now, this question is too vague to pursue in a systematic fashion, so we had to slice it into smaller and more objective chunks. This sectioning is presented in Table 2.

The research question is one of the most important steps in planning a Systematic Literature Review, but it cannot be entered into a library's search box. Therefore, we have to define our search terms before we can make any effort of answering our questions.

3.3. Search Query Definition, Library Selection and Filter Definition

In the case of this study, the search terms were selected in order to purposefuly maintain a broad scope, so that we could retrieve a high number of relevant studies. The selected search terms were: **DOAS atmospher* tomography**[1]. The search query was entered into 5 academic search engines, as shown in Table 3.

Table 3: *Electronic libraries used in this study.*

Library	**URL**
Google Scholar (GS)	https://scholar.google.com/
Web of Knowledge (WoK)	https://webofknowledge.com
Science Direct (SD)	https://www.sciencedirect.com
IEEE	http://ieeexplore.ieee.org/
AGU Publications (AGU)	http://agupubs.onlinelibrary.wiley.com/hub/

[1]The asterisk acts as a wildcard.

After setting Table 3 libraries, it was time to define our article selection criteria, which are summarised in Table 4. We began with 2 Inclusion Criteria (IC) and 3 Exclusion Criteria. The IC determined that our selected papers would have to be journal articles (thus exluding thesis, white papers, patents and other documents) and that these articles should be on the topic of Tomographic DOAS. The EC dictated that no selected paper should include volcanology studies or satellite data analysis (these have particularities which we do not want to approach in this study) and that no other language than English will be accepted.

During the course of the search, however, we had to include another two EC. The first was included in the Google Scholar search, where we understood that papers from a certain publisher were not accessible. The second came in the subsequent searches, when it became clear that most papers had already been retrieved by the GS search.

Table 4: *Selection filters in use for this study's search.*

	Criterium	**Definition**
Exc. Criteria	EC1	Duplicate in Scholar
	EC2	Non English articles are not accepted
	EC3	Volcanology papers are not accepted
	EC4	Satellite data papers are not accepted
	EC5	CNKI published articles are not accepted
Inc. Criteria	IC1	Results must be articles
	IC2	Results must be about Tomographic DOAS

3.4. Data Extraction Strategy

The data extraction process is a key part of any systematic review, whether an SLR or an MS. It determines how each article is approached with regard to its content, before any information is retrieved. In our case, our strategy took place in two separate moments: an initial screening, in which we would assess contents as expressed by the articles' abstract; and a second moment, in which we performed a full article read. Special attention was given to explicit sections covering our target topics (equipment, algorithm and software).

3.5. Quality Assessment

It is very difficult to assess a paper's quality, and to rank it accordingly. However, for this review in particular, we have decided to follow Souza's

Table 5: *Quality assessment criteria presentation.*

Criterium Type	Criterium (Weight)	Decision Factor	Score
General Criteria	Contribution to this SLR (0,2)	cited in study: more than three times	1
		cited in study: three times	0,75
		cited in study: twice	0,5
		cited in study: once or less	0,25
Specific Criteria	Algorithm description (0,6)	Detailed	1
		Semi-Detailed	0,4
		Mentioned	0,2
		None	0
	Instrument description (0,2)	Detailed	1
		Semi-Detailed	0,4
		Mentioned	0,2
		None	0
	Software Description (0,1)	Mentioned	1
		None	0

approach [26] and adopt a similar evaluation method. Table 5 contains the used criteria.

In our evaluation model, we took into account both general ans specific criteria. The former addresses an article's contributions to our particular SLR; the latter targets the actual content of that article.

In order to measure the contribution of each individual paper to our study (our general criterium), we have assessed its number of citations in all the other selected papers. This is a valid measurement of a papers impact in the study, but it might become difficult to implement if a high number of articles are selected for the final stage. Contentwise (specific criteria), we have defined our scoring model according to the Research Question separation explained in Subsection 3.2.

In our study's case, distinction between Specific and General was not sufficient to adequately separate scores according to importance. It was necessary to introduce scoring weights for that end. These weights are also shown in Table 5 and were set according to the goals of our SLR, meaning that the tomographic element is the most important.

In the end, a paper's total score comes from the formula described by Equation 2.

$$TotalScore = \sum_i w_i \cdot S_i \tag{2}$$

Where S_i and w_i are a paper's score and weight for a given criterium, respectively.

Finally, we shall discuss the different weights given to each criterium and the different ways in which they are evaluated. The most important aspect that we are trying to assess is the algorithm, which defines the whole tomographic process and the results achievable by the studies.

A detailed algorithmic description includes the mathematical basis as well as a complete description of required adaptations, both on the mathematical level and on a conceptual method.

Instrument description is also an important criterium, since it is with it that scientists retrieve the information they will afterwards process tomographically, through the algorithm.

It is sometimes difficult to establish how good an instrument descrition is. A too detailed description can be just as bad as a non-sufficient one, if the equipment options are not correctly presented.

That being said, we have considered a detailed description one that includes explicit mention to the composition of the optical system and its assembly details, together with the analysing hardware (e.g. spectrometers) configuration and capabilities.

The least important of the technical features under evaluation is the software. This is because theoretically, results would be the same independently of the software in use. We have included this feature in the study as a way of identifying if there was some kind of software prevalence in the community. In this study, software is binarily assessed: either the scrutinised study mentions it or not.

Finally, we evaluate the contribution of each article to this study. Since DOAS tomography is a field with a relatively low number of players, it can be expected that there are many cross citations. We have introduced this as a method of measuring an article's relative importance within this mapping study, simply by counting the number of times a cross citation occurs.

4. Conduction

4.1. The Search

SLR guideline literature [14, 28] recommend that the first stage of any Systematic Literature Review be the search for previous literature of this kind, since a recent systematic study may render the execution of a new study disencourageable. In our case, none of the several libraries used appeared to have any article of the sort.

The search terms, derived in Subsection 3.2, were run in all libraries found in Subsection 3.3. The Google Scholar search had the particularity of being run through a specialised software called *Publish or Perish*[8], which allowed the search results to be exported to a comma separated values file, which made the process a lot easier, since it was then possible to work the data directly in a spreadsheet program (Microsoft Excel, in this particular case).

The conduction phase of our study followed the flowchart illustrated by Figure 1. Notice that Google Scholar is the first library to be searched. This is motivated by the fact that the vast majority of the articles were retrieved by Google's academic search engine. In fact, GS-retrieved articles were so predominant that we had to create a special EC, as described in Subsection 3.3.

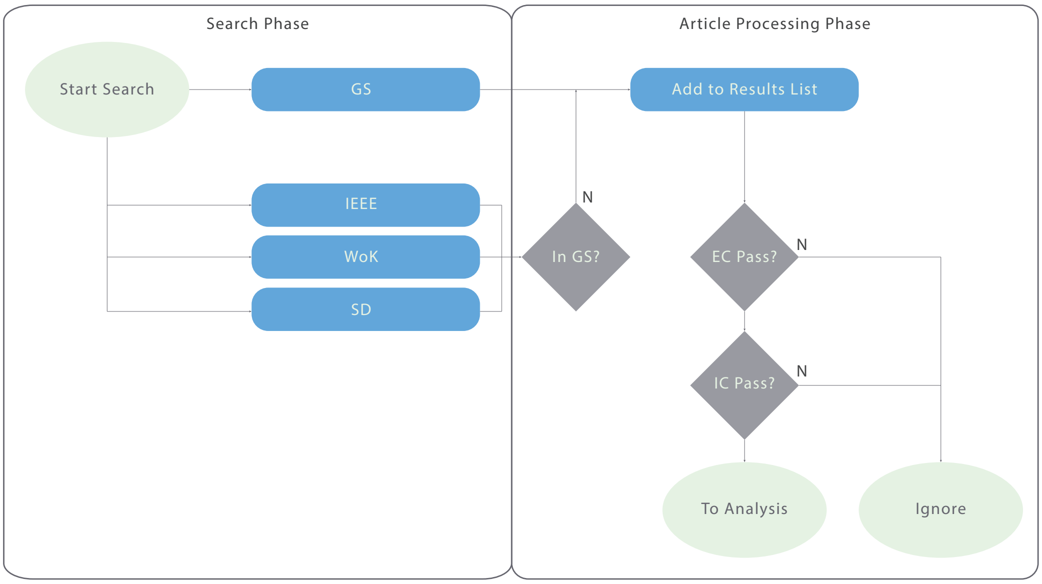

Figure 1: *Conduction stage flowchart. Notice Google Scholar's prevalence.*

4.2. Results and Discussion

4.2.1. Presentation and analysis

Our search returned 732 results, of which 709 were distinct (≈97%). Of these, 601 were journal articles (≈82%). The vast majority of the results came from GS (≈80%, see Figure 2). Selection criteria (Inclusion and Exclusion) application resulted in the exclusion of 701 results (≈99%), thus leaving 8 articles reaching the content analysis stage (the attempt to answer the Research Question). A summary of these findings can be seen in Table 6.

Table 6: *Search results. For a paper to reach the righmost column, which means it is selected, it must verify both IC1 and IC2 as well as none of the EC, ranging from EC1 to EC5.*

		Articles which trigger criteria							
Source	**# Articles**	**IC1**	**IC2**	**EC1**	**EC2**	**EC3**	**EC4**	**EC5**	**Rem. Articles**
GS	576	455	142	-	25	82	53	18	8
IEEE	116	116	1	0	0	1	1	0	0
WoK	14	14	6	13	0	1	1	0	0
SD	10	0	0	0	0	0	0	0	0
AGU	16	1	1	1	1	1	1	0	1
								TOTAL	9

Library	# Results	Percentage
GS	576	78.7%
IEEE	116	15.8%
WoK	14	1.9%
SD	10	1.4%
AGU	16	2.2%

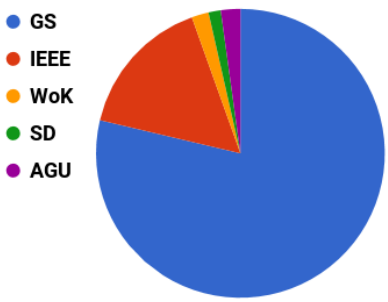

Figure 2: *Results distribution by library.*

Table 7 presents the 8 selected articles. It categorises them with respect to their covered topics and whether they are empirical or theoretical in nature. The same table summarises article scores according to the criteria defined in Subsection 3.5, and presents the the keys with which we will refer to each article from this point forward.

The 8 papers averaged a score of 0,48 and a median score of 0,6. There is a strong difference between the average and the median suggesting that there are some outliers or some kind of clustering. Although this is actually the case, it is statistically irrelevant, given the small size of the sample.

Table 7: *Scoring results for the selected articles. In the second column, a T means the article is theoretical and an E means the article is empirical.*

Key	**Type**	**Alg.**	**Inst.**	**Soft.**	**Cit.**	**Score**
Hartl2006 [7]	T	1	0,4	0	0,5	0,73
Laepple2004 [15]	T	1	0	0	1	0,70
Mettendorf2006 [17]	E	0,4	1	1	0,25	0,57
ODriscoll2003 [18]	T	1	0	0	0,25	0,63
Olaguer2017 [19]	E	0	0,2	0	0,25	0,07
Poehler (unpub) [23]	E	0	0,4	0	0,25	0,11
Pundt2005 [24]	E	0,4	1	1	1	0,64
Stutz2016 [27]	E	0	1	1	0,25	0,33

4.3. Discussion

In this subsection, we will use the 8 articles that were selected in order to try and answer the Research Questions. For clarity, we will approach with respect to the instrument, algorithm and software in a separate manner.

Different articles present data in different ways, and with different levels of detail. This has been taken into account in designing our evaluation method, and it should also be observed when discussing results. Therefore, our general approach in this subsection will be to address the more detailed articles first and then complement that information with what we can gather from the less detailed papers.

4.3.1. Instrument

Instrumentation description is present in 7 of the 8 ([7, 15, 17, 19, 23, 24, 27]) selected articles. Stutz2016 [27], Pundt2005 [24] and Mettendorf2006 [17] present the highest level of detail.

In Stutz2016 [27], the authors used a newly developed Long Path DOAS instrument for the study of atmospheric concentration of Benzene, Toluenes and Xylenes. This instrument's main innovation is its light source, which consists in a double LED (255nm and 265nm) assembly. This system's telescope is a homebuilt telescope with a focal length of 120 cm and a 12 inch diameter aluminum coated main mirror, mounted on a high accuracy motorised pan and tilt unit from Newark Systems. The telescope is used both as emitter and receiver, therefore the system needs a reflector. Stutz used a quartz corner cube reflector array, with an individual reflector diameter of 57 mm and the number of reflector ranging from 10 to 25 (depending on the path length). For detection, the system relied on a UV-enhanced PIXIS 256 CCD detector from Princeton Instruments on an Acton spectrometer with 300 grating and ≈0,3 nm spectral resolution, which was stabilised to -35°C.

Pundt2005 [24] was conducted during the BAB II motorway campaign. The team was working with the goal of performing a tomographic measurement of vehicle polution along a certain motorway between Heidelberg and Mannheim. For that, they used an assembly of two telescopes and eight reflectors, rendering a total of 16 light paths, then used to perform a tomographic reconstruction of the trace gas detection in that region. The telescopes used had a focal length of 150 and 80 cm, with respective diameters of 300 and 200 mm. Both assemblies used Acton spectrometers. One used the Acton 500, with 0,5 nm spectral resolution in the range between 295 and 375 nm; the other used an Acton 300, with 0,4 nm spectral resolution between 295 and 355 nm. In both cases, the sensor used was a 1024 pixe Photo Diode Array (PDA), thermally stabilised at -15°C. The telescopes were pointed towards two towers which beared the reflectors, set at heights of 10, 20, 30 and 40 m from the ground.

In Mettendorf2006 [17], the authors validated two-dimensional LP-DOAS tomography through an indoor experiment. To this end, they have used three multibeam instruments, which consisted in a telescope with a focal length of 1,5 m and 300 mm in diameter, which was also used as emitter and receiver. The system used a broad spectrum Xenon lamp as light source, though no details are given. The experiment assembly included the careful positioning of plane mirrors and 6 cm diameter corner cube reflectors, used to create a total of 39 light paths (13 for each multibeam instrument).

As for the other 4 less detailed instrument description, three (Hartl2006 [7], Poehler [23] and Laepple2004 [15]) are from the same group as Pundt2005 [24] and Mettendorf2006 [17], and therefore use the same or similar hardware. Olaguer2017 [19], on the other hand, is the companion paper of Stutz2016 [27], and therefore gives a description of the same instrumentation, though in a less detailed manner.

4.3.2. Algorithm

The reconstruction algorithm is the most important part of our study, as we already demonstrated by the weight it is given in our quality evaluation model (see Subsection 3.5). Algorithm descriptions are present in 6 of the 8 selected articles: [7, 15, 17, 18, 19, 24]. The most complete descriptions are featured in Hartl2006 [7], Laepple2004 [15] and ODriscoll2003 [18]. Mettendorf2006 [17], Olaguer2017 [19] and Pundt2005 [24] approach the reconstruction algorithms with less emphasis or in a less detailed way.

In Hartl2006 [7], the research team describe their discretisation process, reconstruction methods, grid translation methods and error estimation and quality assessment, with the greatest level of detail being given to the latter.

The paper also focuses in the comparison SIRT and ART results for the test samples, which consisted in up to four Gaussian concentration profiles, which were randomly arranged in a 100x100 (a.u.) test field, in six different geometries and with up to 36 known light paths.

Furthermore, Hartl2006 [7] discusses how the choice of the reconstruction grid affects both the reconstruction error and reconstruction area integrals, the possibility of the existence of background concentration influencing equation constraints and reconstruction results, and how the whole system would behave were its geometry any different, namely regarding light paths and number of telescopes.

The next algorithm-oriented paper is Laepple2004 [15]. In this article, the group discussed several discretisation approaches, their drawbacks and advantages. Still on discretisation, they approach the problem of resolution, and the necessary balance between physical accuracy and the need for *a priori* information which arises from increasing it. Afterwards, the group presents some strategies for solving the linear system that results from discretising the concentration field and how to take error into account.

For their reconstructions, the group chose to adapt ART, SIRT, and SART (see Subsection 2.4). These adaptations were described and detailed in the article's third section, before the error estimation procedures adopted in their case. Finally, the team presents how they chose to optimise reconstruction in several aspects, including the generation of test plumes and optimisation for the BABII campaign, which was the parent project of this article.

ODriscoll2003 [18] also covers the algorithm extensively. While this paper is considerably shorter that the previous two, it provides a detailed (on an iteration basis) description for ART ani SIRT (see Subsection 2.4). In addition, and perhaps of greater interest, the paper's authors suggest a different approach to solving the reconstruction matrix, different from the algebric methods already presented: an evolutionary algorithm.

An evolutionary algorithm is a mathematical method of solving complex problems, which mimics or is in any form based on the process of natural selection. These algorithms have, according to the paper's authors and their references, been shown to be extraordinarily powerful.

The research team have applied a Differential Evolution algorithm to the reconstruction process and provide a detailed description of how they have done this.

The other two articles which mention the algorithm are Mettendorf2006 [17] and Pundt2005 [24]. Both these studies were conducted under the same project as Laepple2004 [15] and Hartl2006 [7] and therefore their algorithm descriptions and methods draw heavily on these two studies.

4.3.3. Software

Of the 8 selected articles, only 3 mention the software used. Even these, do not go into any detail of the reasons that led to that specific usage.

In Mettendorf2006 [17], the team used TOMOLAB for the calculation of the modelled column densities of their experiment. In Pundt2005 [24], spectral analysis was performed using the *MFC Software*. Finally, Stutz2016 [27] used the DOASIS software for control and automation purposes, and does not explicitly mention its use for spectral analysis purposes, although this is likely.

4.3.4. General Observations

While this is not a part of the discussion *per se*, we believe it makes sense to make some general observations about the data which wwe had to analyse.

The first important mention is the BABII campaign. This study, which ran in 2001 and aimed to quantify polution from the A656 motorway between Heidelberg and Mannheim produced a significant part of the literature which we analysed.

Another point which should be addressed is that all DOAS tomography efforts detected in this search were based on active DOAS technology. This only means that the DOAS systems all employed an artificial light as a light source.

A final remark is due to the prevalence of algebric methods for solving the discretisation and reconstruction problem, namely ART, SART and SIRT.

4.4. Validity Threats

When writing an MS or an SLR, authors always have to analyse their findings and methods in order to mitigate potential sources of error or lack of validity. This is called a validity threat analysis.

There are two main families of validity threats. They can be internal, i.e., they come from the methods employed used in conducting the study; or external, which means that the threat comes from the applicability (or lack thereof) of the effects observed in the study, outside of its scope.

On the level of internal validity of our study, two main observations come to mind:

Relevant papers left out The very low number of found studies could be an indication that our inclusion and exclusion filters were set in a too restrictive manner.

It could also happen that some relevant papers were not found due to being written in such a way that the libraries' search engines did not find them with our search phrase. This same problem would also occur if for some reason, an important library was left out of the study, and therefore not searched.

We mitigate all these risks by selecting a purposefuly broad search phrase, by using powerful general search engines (eg. Google Scholar) and by running several undocumented test-runs with other search phrases.

A common strategy used for tackling this kind of threat is to extend the study through snowballing. In our case, we have opted to not perform this operation because of the very high cross-reference pattern between the found studies.

Quality of selected papers While it is true that we do not have any control over the quality of the articles rendered by the search engines, and there is no standard regarding it, we must address the issue that it entails. We have tried to mitigate this risk, as far as we can, by using strict and strong selection criteria in systematic fashion (see Section 3).

On the external threat plane, we contend with the applicability of our findings outside our study. We have tackled this issue by trying to remaining focused only to the techonologic aspect of the Tomographic DOAS technique, both in respect to its instrumentation and to the mathematical methods involved.

With this in mind, and even if the internal validity threats were all verifiably concerning, this study's finding are of great use to anyone wanting to understand how the field is working or wishing to design and build an analysis system.

5. Conclusions

The essential goal of this MS was to assess the technological sttaus of the tomographic DOAS technique as described in the relevant academic literature.

By performing a systematic search using the phrases and libraries enumerated in Section 3, we have retrieved more than 700 articles. The elimination process took place through the application of inclusion and exclusion criteria, as described in full in Subsection 3.3.

In the end, 8 articles were identified as relevant. There are several possible justifications for such a low number of retrieved articles. Some of those reasons are addressed in Subsection 4.4. Mostly, we believe that DOAS tomography is a relatively new field of study, which has not yet been sufficiently explored, and that results in a small *corpus* of literature.

Our analysis was performed on three distinct levels: **algorithms**, **hardware** and **software**. We have found that, while there are commonalities amongst almost all papers (such as the fact that they are all active DOAS applications), on the hardware and software planes, there is no *standard model* for the used devices. On the algorithm level, however, and due to data quantity restrictions related to the low number of used projections (several tens), iterative reconstruction methods (namely ART) are almost universal.

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