Linköping University | Department of Computer and Information Science

Master's thesis, 30 ECTS | Statistics and Machine Learning

2021 | LIU-IDA/LITH-EX-A--2021/001--SE

Improving the identification of nitrogen oxides and ammonia using frequency modulation in gas sensors

– **DRAFT**

Förbättra identifieringen av kväveoxider och ammoniak med frekvensmodulering i gassensorer

Marcos Freitas Mourão dos Santos

Supervisor : Annika Tillander
Examiner : José M. Peña

External supervisor : Mike Andersson

LINKÖPING UNIVERSITY

Linköpings universitet
SE–581 83 Linköping
+46 13 28 10 00 , www.liu.se

Upphovsrätt

Copyright

Abstract

The abstract resides in file `Abstract.tex`. Here you should write a short summary of your work.

Acknowledgments

Acknowledgments.tex

Contents

Abstract **iii**

Acknowledgments **iv**

Contents **v**

Acronyms **1**

1 Introduction **2**
1.1 Motivation 2
1.2 Aim 3
1.3 Research questions 3

2 Theory **4**

3 Data **5**

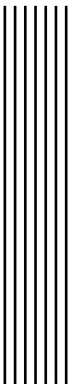
4 Method **6**

5 Results **7**

6 Discussion **8**
6.1 Results 8
6.2 Method 8
6.3 The work in a wider context 9

7 Conclusion **10**

Bibliography **11**



Acronyms

GBCO Gate Bias Cycled Operation. 3

PLSR Partial Least Squares Regression. 3

SCR Selective Catalytic Reduction. 2

SiC-FET Silicon Carbide Field Effect Transistor. 3

TCO Temperature Cycled Operation. 3

1 Introduction

1.1 Motivation

Nitric Oxide (NO) and Nitrogen Dioxide (NO_2), commonly referred together as NO_x, are hazardous gases to the environment and to humans. Its main sources are combustion processes in transportation, and industrial processes such as (but not limited to) auto mobiles, trucks, boats, industrial boilers, turbines, etc. [7].

NO_x exposure to humans can cause respiratory illnesses such bronchitis, emphysema and can worsen heart disease [4]. Environmentally, NO_x are deemed precursors of adverse phenomena such as smog, acid rain, and the depletion of ozone (O_3) [1]. It is of high interest, therefore, to reduce NO_x emissions.

One well studied and successful method of reducing emissions is Selective Catalytic Reduction (SCR), which consists in the reduction of NO_x by ammonia (NH3) into nitrogen gas (N2) and water (H2O) [5], both harmless components. The process is based in the following reactions [5]:

$$4\,NH_3 + 4\,NO + O_2 \longrightarrow 4\,N_2 + 6\,H_2O$$

$$2\,NH_3 + NO + NO_2 \longrightarrow 2\,N_2 + 3\,H_2O$$

$$8\,NH_3 + 6\,NO_2 \longrightarrow 7\,N_2 + 12\,H_2O$$

One key element in these reactions, however, is the amount of ammonia dosed into the SCR systems. Ammonia itself is hazardous to humans, causing skin and respiratory irritation, among other illnesses [2]. More importantly, ammonia is one of the main sources of nitrogen pollution and it has direct negative impact on biodiversity via nitrogen deposition in soil and water [6]. Hence it is also desired to keep ammonia emissions to a minimum. Too much ammonia in the SCR catalyst will guarantee NO_x reduction at the expense of undesired ammonia emissions. Concurrently, too little ammonia will impede SCR to occur properly, beating the purpose of the catalyst and as a consequence, undesired NO_x emissions.

To monitor gasses concentrations, chemical sensors are deployed, one of which is the Silicon Carbide Field Effect Transistor (SiC-FET). The identification and quantification of gasses is normally achieved through multiple sensor in so called sensor arrays. Ideally each sensor in the array needs to have different responses to different compounds [3]. The deployment of multiple sensors, on the other hand, proves itself cumbersome due to the increased chances of failure, and decalibration of the system should one or multiple sensors be replaced [3].

One solution to this problem is the cycled operation of one single sensor, referred as virtual multi-sensor [3]. By cycling the working point parameters of the sensor, different substances react differently in the sensor surface, which in turn produces different responses. Temperature Cycled Operation (TCO), Gate Bias Cycled Operation (GBCO), and the combination of the two have been proven to increase selectivity of SiC-FET sensors [3].

1.2 Aim

The aim of this thesis is to investigate different regression methods, namely: Partial Least Squares Regression (PLSR), Ridge Regression and (neural nets XXXX - TENTATIVE), and their fit to correctly quantify gas mixtures such NO_x and Ammonia subjected to sensor frequency modulation.

1.3 Research questions

1. Can frequency modulation be used to simultaneously quantify NO_x and Ammonia?
2. Which method yields best predictions of gas concentrations?

2 Theory

The main purpose of this chapter is to make it obvious for the reader that the report authors have made an effort to read up on related research and other information of relevance for the research questions. It is a question of trust. Can I as a reader rely on what the authors are saying? If it is obvious that the authors know the topic area well and clearly present their lessons learned, it raises the perceived quality of the entire report.

After having read the theory chapter it shall be obvious for the reader that the research questions are both well formulated and relevant.

The chapter must contain theory of use for the intended study, both in terms of technique and method. If a final thesis project is about the development of a new search engine for a certain application domain, the theory must bring up related work on search algorithms and related techniques, but also methods for evaluating search engines, including performance measures such as precision, accuracy and recall.

The chapter shall be structured thematically, not per author. A good approach to making a review of scientific literature is to use *Google Scholar* (which also has the useful function *Cite*). By iterating between searching for articles and reading abstracts to find new terms to guide further searches, it is fairly straight forward to locate good and relevant information, such as [**test**].

Having found a relevant article one can use the function for viewing other articles that have cited this particular article, and also go through the article's own reference list. Among these articles on can often find other interesting articles and thus proceed further.

It can also be a good idea to consider which sources seem most relevant for the problem area at hand. Are there any special conference or journal that often occurs one can search in more detail in lists of published articles from these venues in particular. One can also search for the web sites of important authors and investigate what they have published in general.

This chapter is called either *Theory, Related Work*, or *Related Research*. Check with your supervisor.

3 Data

4 Method

In this chapter, the method is described in a way which shows how the work was actually carried out. The description must be precise and well thought through. Consider the scientific term replicability. Replicability means that someone reading a scientific report should be able to follow the method description and then carry out the same study and check whether the results obtained are similar. Achieving replicability is not always relevant, but precision and clarity is.

Sometimes the work is separated into different parts, e.g. pre-study, implementation and evaluation. In such cases it is recommended that the method chapter is structured accordingly with suitable named sub-headings.

5 Results

This chapter presents the results. Note that the results are presented factually, striving for objectivity as far as possible. The results shall not be analyzed, discussed or evaluated. This is left for the discussion chapter.

In case the method chapter has been divided into subheadings such as pre-study, implementation and evaluation, the result chapter should have the same sub-headings. This gives a clear structure and makes the chapter easier to write.

In case results are presented from a process (e.g. an implementation process), the main decisions made during the process must be clearly presented and justified. Normally, alternative attempts, etc, have already been described in the theory chapter, making it possible to refer to it as part of the justification.

6 Discussion

This chapter contains the following sub-headings.

6.1 Results

Are there anything in the results that stand out and need be analyzed and commented on? How do the results relate to the material covered in the theory chapter? What does the theory imply about the meaning of the results? For example, what does it mean that a certain system got a certain numeric value in a usability evaluation; how good or bad is it? Is there something in the results that is unexpected based on the literature review, or is everything as one would theoretically expect?

6.2 Method

This is where the applied method is discussed and criticized. Taking a self-critical stance to the method used is an important part of the scientific approach.

A study is rarely perfect. There are almost always things one could have done differently if the study could be repeated or with extra resources. Go through the most important limitations with your method and discuss potential consequences for the results. Connect back to the method theory presented in the theory chapter. Refer explicitly to relevant sources.

The discussion shall also demonstrate an awareness of methodological concepts such as replicability, reliability, and validity. The concept of replicability has already been discussed in the Method chapter (4). Reliability is a term for whether one can expect to get the same results if a study is repeated with the same method. A study with a high degree of reliability has a large probability of leading to similar results if repeated. The concept of validity is, somewhat simplified, concerned with whether a performed measurement actually measures what one thinks is being measured. A study with a high degree of validity thus has a high level of credibility. A discussion of these concepts must be transferred to the actual context of the study.

The method discussion shall also contain a paragraph of source criticism. This is where the authors' point of view on the use and selection of sources is described.

In certain contexts it may be the case that the most relevant information for the study is not to be found in scientific literature but rather with individual software developers and open source projects. It must then be clearly stated that efforts have been made to gain access to this information, e.g. by direct communication with developers and/or through discussion forums, etc. Efforts must also be made to indicate the lack of relevant research literature. The precise manner of such investigations must be clearly specified in a method section. The paragraph on source criticism must critically discuss these approaches.

Usually however, there are always relevant related research. If not about the actual research questions, there is certainly important information about the domain under study.

6.3 The work in a wider context

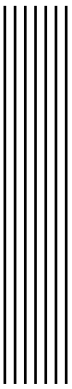
There must be a section discussing ethical and societal aspects related to the work. This is important for the authors to demonstrate a professional maturity and also for achieving the education goals. If the work, for some reason, completely lacks a connection to ethical or societal aspects this must be explicitly stated and justified in the section Delimitations in the introduction chapter.

In the discussion chapter, one must explicitly refer to sources relevant to the discussion.

7 Conclusion

This chapter contains a summarization of the purpose and the research questions. To what extent has the aim been achieved, and what are the answers to the research questions?

The consequences for the target audience (and possibly for researchers and practitioners) must also be described. There should be a section on future work where ideas for continued work are described. If the conclusion chapter contains such a section, the ideas described therein must be concrete and well thought through.



Bibliography

[1] R. Alberto Bernabeo, K. Webster, and M. Onofri. "Health and Environmental Impacts of Nox: An Ultra- Low Level of Nox (Oxides of Nitrogen) Achievable with A New Technology." In: *Global Journal of Engineering Sciences* 3 (), pp. 2–7. DOI: 10.33552/gjes.2019.02.000540.

[2] ASTDR. "Sheet for ammonia published by the Agency for Toxic Substance and Disease Registry (ASTDR)." In: 2672 (2004), pp. 1–18. URL: https://www.atsdr.cdc.gov/MHMI/mmg126.pdf%5C%0Ahttps://www.atsdr.cdc.gov/mmg/mmg.asp?id=7&tid=2#bookmark02.

[3] Manuel Bastuck. "Improving the performance of gas sensor systems with advanced data evaluation, operation, and calibration methods." PhD thesis. Jan. 2019, p. 267.

[4] Thirupathi Boningari and Panagiotis G. Smirniotis. "Impact of nitrogen oxides on the environment and human health: Mn-based materials for the NOx abatement." In: *Current Opinion in Chemical Engineering* 13.x (2016), pp. 133–141. ISSN: 22113398. DOI: 10.1016/j.coche.2016.09.004. URL: http://dx.doi.org/10.1016/j.coche.2016.09.004.

[5] Pio Forzatti. "Present status and perspectives in de-NOx SCR catalysis." In: *Applied Catalysis A: General* 222.1 (2001). Celebration Issue, pp. 221–236. ISSN: 0926-860X. DOI: https://doi.org/10.1016/S0926-860X(01)00832-8. URL: https://www.sciencedirect.com/science/article/pii/S0926860X01008328.

[6] Susan Guthrie, Sarah Giles, Fay Dunkerley, Hadeel Tabaqchali, Amelia Harshfield, Becky Ioppolo, and Catriona Manville. *Impact of ammonia emissions from agriculture on biodiversity: An evidence synthesis*. Santa Monica, CA: RAND Corporation, 2018. DOI: 10.7249/RR2695.

[7] USEPA. *Nitrogen Oxides Control Regulations*. https://www3.epa.gov/region1/airquality/nox.html. Accessed 2021-02-09. 2019.