Improving the identification of nitrogen oxides and ammonia using frequency modulation in sensors via multivariate statistical analysis of sensor data - FIRST DRAFT

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1 Introduction

1.1 Background

TODO: list of acronyms, chemical formulas correct formatting, frequency modulation, images, adjust line /paragraph spacing, change document-class to thesis template, reference alignment

Note to (internal) supervisor. As this topic is very chemistry/physics heavy, I tried to summarize its main ideas in a very concise way to avoid long (and somewhat out of scope) text. Should I keep it like this or ”go deeper” in the chemistry/physics?

Nitric Oxide (NO) and Nitrogen Dioxide (NO2), commonly referred together as NOx, 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. [USEPA, 2019].

NOx exposure to humans can cause respiratory illnesses such bronchitis, emphysema and can worsen heart disease [Boningari and Smirniotis, 2016]. Environmentally, NOx are deemed precursors of adverse phenomena such as smog, acid rain, and the depletion of ozone (O3) [Alberto Bernabeo et al., 2019]. It is of high interest, therefore, to reduce NOx emissions.

One well studied and successful method of reducing emissions is Selective Catalytic Reduction (SCR), which consists in the reduction of NOx by ammonia (NH3) into nitrogen gas (N2) and water (H2O) [Forzatti, 2001], both harmless components. The process is based in the following reactions [Forzatti, 2001]:

4NH3 + 4NO + O2 $\rightarrow$ 4N2 + 6H2O

2NH3 + NO + NO2 $\rightarrow$ 2N2 + 3H2O

8NH3 + 6NO2 $\rightarrow$ 7N2 + 12H2O

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 [ASTDR, 2004]. 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 [Guthrie et al., 2018]. Hence it is also desired to keep ammonia emissions to a minimum. Too much ammonia in the SCR catalyst will guarantee NOx 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 NOx emissions.

To monitor gasses concentrations, chemical sensors are deployed, one of which is the Silicone 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 [Bastuck, 2019].

Figure 1: SiC-FET sensor. Source: [Bastuck, 2019]

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 [Bastuck, 2019].

One solution to this problem is the cycled operation of one single sensor, referred as virtual multi-sensor [Bastuck, 2019]. 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 [Bastuck, 2019].

To be added: more information about SIC-FET Sensor, Temperature cycling, Frequency cycling.

1.2 Objectives - TENTATIVE

- Can frequency modulation be used to improve simultaneous identification of NO/NO2/NH3?
- Investigate influence of frequency modulation on identification of different gas species.

- Compare results to previous work on simultaneous monitoring of NOx/NH3.
- Investigate conceptually different regression methods on gas species separation.
- Try to estimate the effects on emission reduction in real application.

2 Data

2.1 Data Sources

The measurements were made at correct lab name in Linköping University using a gas mixing system controlled by electronic valves.

Add details about experimental set up

2.2 Raw Data

The raw data consists of the sensor response, measured in μA for different combinations of NO, NO2 and NH3. Each gas has three different possible concentrations: 25, 50 and 100 ppm. All possible configurations of gas mixtures were tested in constant temperature (specify what temperature.) and submitted to the same frequency cycle regimen (specify regimen), totalling to 27 different cycles. Each cycle was run for approximately 1300 time steps. Figure 2 below shows the sensor response to the mixture of NO2/NO/NH3 of 100/25/50ppm.

2.3 Secondary Data

tbd.

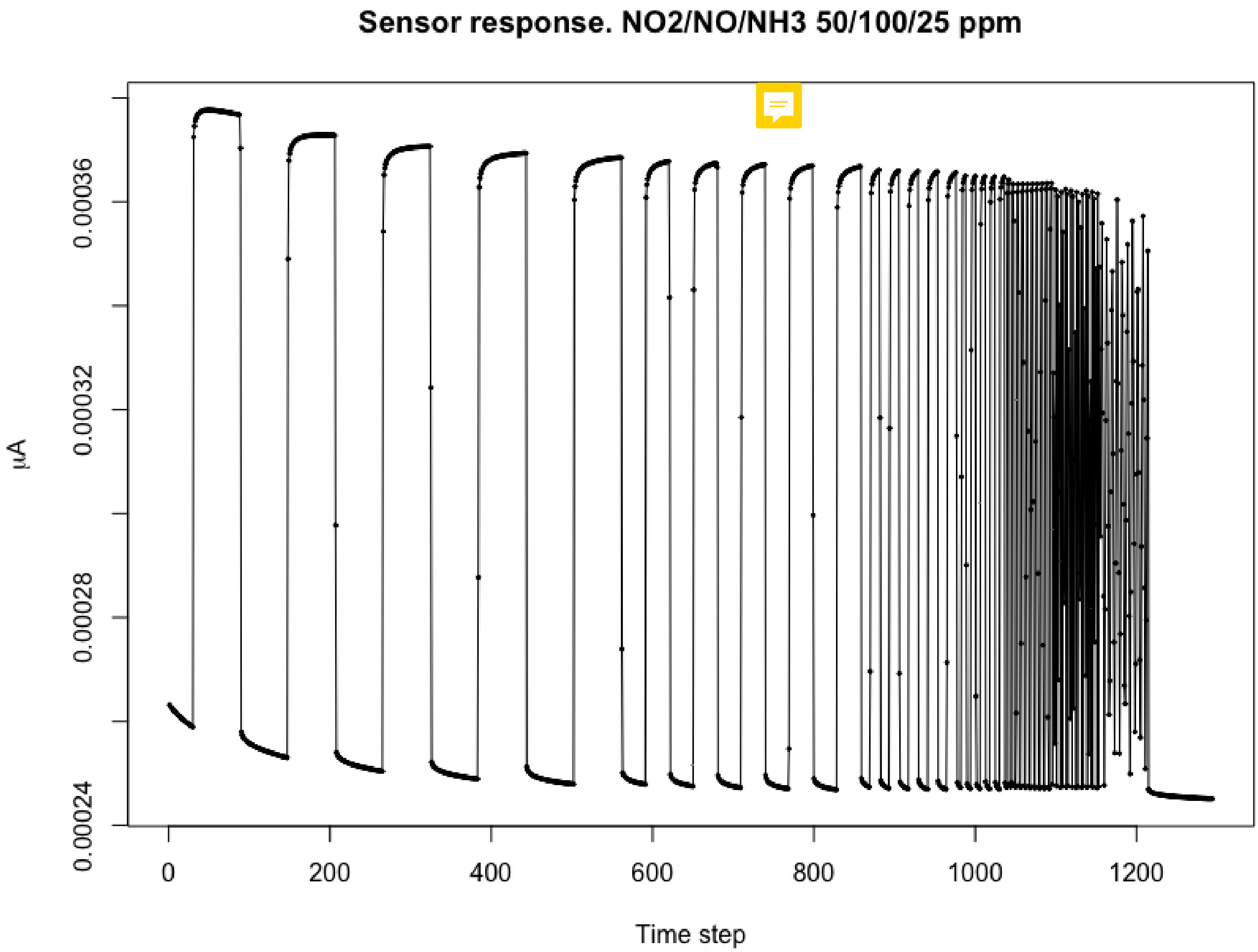

Figure 2: Sensor response for gas mixture 100/25/50 ppm of NO2/NO/NH3

References

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