Machine learning-based NO2 estimation from seagoing ships using TROPOMI/S5P satellite data

Kurchaba, S.

Chapter 1

Introduction

Air pollution ranks among the most pressing challenges in our society. Decades of research have proven a strong adversarial effect of air pollution on human health, the vitality of ecosystems, the state of the atmosphere, and climate change [16, 54, 83, 84]. At the same time, according to the World Health Organization (WHO), 9 out of 10 people currently breathe the polluted air. Moreover, due to the continuous urbanization [98], industrialization, and economic development, the number of potential sources of air pollution is dramatically increasing [3, 87, 83, 111].

One of the most harmful components of air pollution are nitrogen oxides gases ($NO_x \approx NO + NO_2$). These gases play an important role in the destruction of the atmospheric ozone [25]. In addition, anthropogenic NO_x is known to be one of the main precursors of photochemical smog [46, 82], whose harmful effects include aggravation of asthmatic attacks, irritation of eyes and throats of humans and animals, reduction of visibility, damage of the structure of plants and materials [100, 66]. Anthropogenic sources of NO_x include industrial emissions, biomass burning, and emissions from vehicle transport. One of the strongest sources of anthropogenic emission of NO_x is the industry of international shipping. The NO_x is produced in a ship engine through the combustion process, where nitrogen in the air reacts with oxygen, forming nitrogen oxides, primarily in the form of nitric oxide (NO). Subsequently, atmospheric conditions and chemical reactions transform NO into nitrogen dioxide (NO_2), a more reactive and harmful component of NO_x emissions. The global contribution of the shipping industry to the emissions of NO_x is estimated to vary between 15% – 35% [24, 52], causing approximately 60,000 premature deaths annually [23]. For the Netherlands, the contribution of the shipping industry is estimated to be around 10% [48]. While

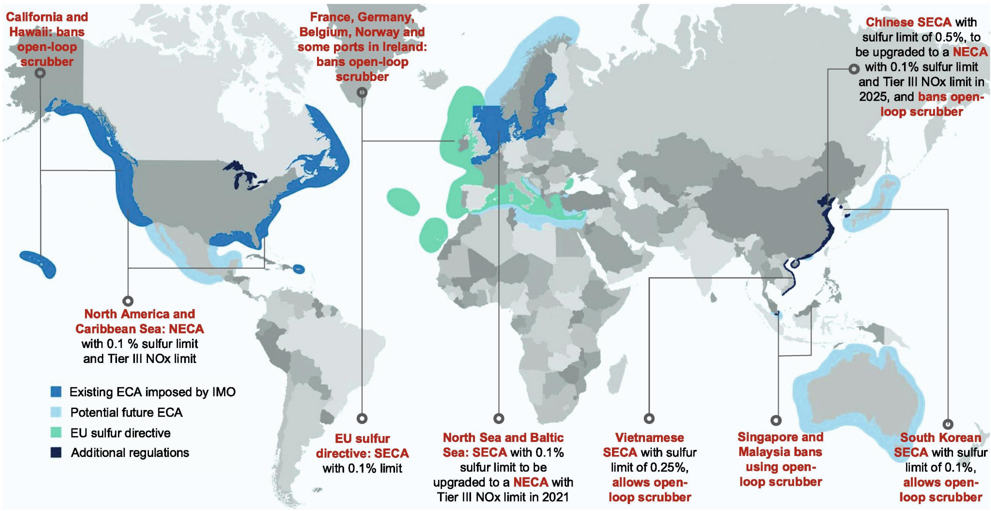

Figure 1.1: Map of ECA's restrictions. Source: [113].

over the last 20 years, the pollution produced by power plants, the industry sector, and cars has been constantly decreasing, the impact of maritime transport continues to grow [12]. This causes a big societal pressure, which calls for a collective effort for efficient regulation and monitoring of emissions from ships towards reducing the negative impact of the industry.

1.1 Ship emission monitoring

In 1997, aiming at the reduction of the negative impact on human health, the International Maritime Organisation (IMO) amended Annex VI to the International Convention for the Prevention of Pollution from Ships (MARPOL). This annex sets standards on sulfur dioxide and nitrogen oxides emissions from ship exhausts [50]. The amendments include the installation of emission control areas (ECAs) within which the emission constraints for ships operating in these areas are established and then tightened step-by-step. The map of currently established and considered ECAs is depicted in Figure 1.1. Within ECA regions, we distinguish nitrogen and sulfur emission control areas (NECA and SECA respectively). The latest step that was turned into force as a part of IMO directives is an 80% reduction of NO_x emission for diesel engines of newly-built ships operating in the Baltic and North Sea [51]. Compliance with these regulations requires shipowners and operators to invest in cleaner, more expensive technologies (e.g. installation of a selective catalytic reduction (SCR) system, which converts harmful gases into inert nitrogen and water vapor). The responsibility for the enforcement of IMO regulations is shared between the country where a given ship is registered and the authorities of the port where the ship operates. In the Netherlands, this is the Human Environment and Transport Inspectorate (ILT). Given the legislation, the responsibilities of the inspectorate are as follows: 1) Monitoring of emissions coming from ships to assess the effects of the legislation; 2) Verification of compliance of individual ships. The performance of neither of the above-mentioned is possible without efficient measurements of real-world emissions. Hence the support of ILT of the research presented here.

However, monitoring of ship emissions on a large scale is a challenging task. For instance, the methods currently used by port state authorities are checks on engine room logs and bunker delivery notes, or chemical analysis of fuel samples. Such practices, however, can be applied to only a limited number of ships. Other applied methods are on-board measurements at exhaust pipes [4], land- or ship-based downwind measurements using sniffer techniques [66, 81], and the DOAS (differential optical absorption spectroscopy) approach [73, 88, 59]. Alternatively, ship plume measurements are performed from airborne platforms like helicopters, small aircraft, and drones [102, 103]. Mobile platforms often measure pollutant ratios during plume transects [7] or use the DOAS technique for remote optical sensing [9]. All these methods require proximity to the ships under surveillance, are applied sporadically, and are too costly for monitoring the entire shipping fleet. Moreover, since such measurement stations are usually located at the entrance of the ports, the data collected with such methods provide limited information on how much the selected ships emit outside ports. As a result, there is currently no effective method for comprehensive and cost-efficient large-scale ship emission monitoring.

1.2 Satellite observations

A potential solution efficient for ship emission monitoring on a global scale is the application of satellite observations [90]. For more than a decade scientists have been using the available satellite data to quantify the NO_x emission produced by the shipping industry. For instance, using the measurements from the Global Ozone Monitoring Experiment (GOME) [17] instrument onboard the second European Remote Sensing satellite (ERS-2), the authors estimated the NO_2 emission levels above the shipping lane between Sri Lanka and Indonesia [8]. With the images from the SCanning Imaging

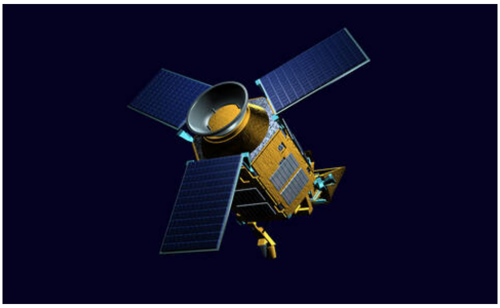

Figure 1.2: Sentinel-5 Precursor satellite. Credit image ESA 2017.

Absorption spectroMeter for Atmospheric CartograpHY (SCIAMACHY) [13] onboard the ENVIronmental SATellite (Envisat) mission, traces from the shipping industry over the Red Sea were quantified [85]. Finally, data from the Ozone Monitoring Instrument (OMI) [69] aboard the NASA Aura spacecraft was used to visualize the NO_x emission inventory of shipping in the Baltic Sea [106]. The obtained results were further associated with the temporal patterns of global economic activity [26, 12]. Nevertheless, all the above-mentioned studies were based on multi-month data averaging, which was necessary to perform in order to reduce the signal-to-noise ratio of the satellite measurements and enable distinguishability of NO_x traces along the shipping lanes. The low spatial resolution of the satellites did not allow for the distinction of ship plumes from individual ships on a daily basis.

The game changer in high-resolution atmospheric measurements is the TROPOspheric Monitoring Instrument (TROPOMI) onboard the Copernicus Sentinel-5 Precursor (TROPOMI/S5P) satellite (illustration: Figure 1.2). Launched in 2017, the TROPOMI/S5P creates daily global maps of atmospheric substances relevant to air quality and climate monitoring [1]. More importantly, the instrument has a significantly higher spatial resolution than all its predecessors (GOME: 40×320 km^2, SCIAMACHY: 30×60 km^2, OMI: 13×25 km^2, TROPOMI: 3.5×5.5 km^2). The TROPOMI instrument measures an extensive list of trace gases, including NO_2. Since the NO_2 gas is the product of photo-chemical reactions of NO_x emitted by ships, it can be utilized for ship emission monitoring. As reported in [41], the spatial resolution of the TROPOMI instrument is high enough to distinguish some of the NO_2 plumes produced by individual ships. This study, however, focused on the largest ships in the area, as the NO_2 traces of most of the ships seemed not sufficiently stronger than the background concentrations. In addition, the presented approach involves multiple manual steps, which prevents its application on a large scale [41].

1.3 Machine learning

In order to increase the sensitivity of ship plume detection, in this thesis, we propose to address the problem with machine learning techniques that have proven very valuable in many domains. Machine learning is a computational paradigm that enables the automatic extraction of complex patterns and relationships in data, not only significantly reducing the human effort required, but also facilitating finding patterns that are otherwise unnoticeable to a human eye. A general definition of machine learning was proposed by Tom Mitchell in 1997 [74]. It goes as follows:

Definition 1.1. Machine learning is the study of computer algorithms that improve automatically through experience. An algorithm is said to learn from experience E with respect to task T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E.

Today, machine learning algorithms have demonstrated their efficiency in various fields of everyday life and science. The list of application domains that were revolutionized by machine learning includes health care (disease diagnosis [6], drug discovery [99]), finance (algorithmic trading [79], fraud detection [71]), computer vision (facial recognition [108], autonomous vehicles [65]), education (adaptive learning systems [56], automated feedback [28]), space exploration (spacecraft control and navigation [95], data processing for remote sensing missions [112]), and many more. In the domain of Earth observation, the list of tasks to which machine learning algorithms have made ground-breaking contributions includes (non-exhaustively) land cover classification, identification of crop diseases, algorithms for the optimization of the retrieval of satellite measurements, flood prediction, and optimization of computer code performance [92, 97, 68, 15, 91].

Different applications and tasks require different types of machine learning algorithms, such as supervised, semi-supervised, unsupervised, or reinforcement learning. In the domain of Earth observation, one of the most often used types of machine learning algorithm is supervised learning [37]. In supervised learning, we aim to learn a function to predict the output Y for a feature vector X. The learning process uses pairs of feature vectors and the corresponding outputs that are given as a training set (the Experience). Depending on the type of output variable, the supervised learning task can further be split into classification (categorical output variable) and regression (continuous output variable).

Emerging studies show the potential of supervised learning techniques for the analysis and information extraction from TROPOMI data. For instance, researchers applied a multivariate regression model to estimate the NO_2 emission rate over Germany [20], and O_3 concentrations in California [110]. Furthermore, classification models were used to automatically detect images containing NO_2 [38] or CH_4 [89] plumes from super-emitters, scanning the TROPOMI data around the globe. Analyzing the above-mentioned studies, we see two ways of representing TROPOMI measurements to a machine-learning algorithm, depending on the problem addressed. That is, in terms of a two-dimensional grid (an image), or a set of one-dimensional data features, calculated based on the measurement values for a specific area of interest. The former enables the application of techniques originating from the fields of computer vision or image processing (i.e. kernel-based filters, convolution neural networks, etc.), while the latter is more suited for the usage of multivariate techniques, combining the TROPOMI measurements with other data sources.

In this thesis, we explore the possibilities of estimation of the NO_2 emissions from individual ships using TROPOMI data. The emissions produced by a ship, if strong enough, will be registered by a TROPOMI sensor as an image of a plume. However, to estimate emissions produced by a certain individual ship, the information contained in the TROPOMI measurement is not sufficient. Other pieces of necessary information are the position of the ship, the speed, and dimensions of the ship, and the direction and speed of the wind. To efficiently exploit all the necessary sources of data, we will mostly focus on the application of multivariate supervised machine learning, while the spatial characteristics of the data will be utilized for image enhancement.

1.4 Research questions

The objective of this thesis is to pave the way toward the application of the TROPOMI instrument data for the monitoring of ship compliance with the regulations of IMO. The overarching research question addressed in this thesis can be formulated as follows:

Is it possible to use TROPOMI/S5P instrument data to monitor NO_2 emissions from individual seagoing ships?

We address this overall question step by step by answering the following list of intermediate research questions:

RQ1: *What is the minimum speed and length of a seagoing ship so that the NO_2 plume from it can be detected with a detection system using TROPOMI data?*

To understand the potential of the TROPOMI instrument for ship emission monitoring, it is crucial to estimate the required strength of the emitter (in this case, a ship) for the detection of its NO_2 plumes. With the detection system, we refer to a sequence of steps needed for the automatic identification of NO_2 plumes from a ship on a TROPOMI image patch. The first step of this sequence is a measurement performed by the TROPOMI sensor. The last step is an automated detection of a plume on an image patch using machine learning models. We propose to estimate the detection capabilities of the TROPOMI data-based detection system using parameters such as speed and length of the ship, known to be reliable indicators of ship emission potential.

RQ2: *To what extent can the detectability of NO_2 plumes be improved if only the biggest emitters are taken into account?*
It is not possible to monitor all ships with a detection system based on TROPOMI data – there is a system sensitivity limit. There also will be a set of ships for which detection is possible, although difficult. Finally, there will be a set of the biggest emitters, from which the plumes are clearly the easiest to detect. Another example of the biggest emitters is when several ships are sailing in proximity to each other. To establish the baseline for the current possibilities of the application of a detection system using the data from the TROPOMI instrument for ship emission monitoring, the potential quality of detection of plumes produced by those biggest emitters should be evaluated separately.

RQ3: *Is there a potential for improvement of detectability of NO_2 plumes from the slow/small ships if more data were used to train the used classification model?*
Since the application of machine learning is an important part of the studied detection system of ship NO_2 plumes, the factor of data availability plays an important role in establishing the sensitivity limits of this system. The noisier the pattern we would like to detect, the more data are required for the training of a machine learning model. This will be especially relevant for ships that are just above the sensitivity limit of the detection system. Therefore, we would like to understand to which extent the addition of training data can help with the detection of the noisiest patterns.

RQ4: *How to assign a TROPOMI signal associated with a certain plume to a potential emitting ship?*
A characteristic feature of a ship as an emitter is the fact that it moves continuously. In addition to the movement of a ship, the plume emitted by it at a certain moment will gradually move in accordance with the direction and speed of the wind. These factors make the process of association of the detected plume with a ship emitter a non-trivial task. The task, however, is a necessary step in order to be able to use the TROPOMI data for the performance of the monitoring of emissions from individual ships.

RQ5: *To what extent can the NO_2 plumes be segmented in the TROPOMI data using a simple thresholding method?*
Segmentation of NO_2 plumes from individual ships using data from satellite-based sensors has not been performed before (because of the too-low spatial resolution of the previous satellite-based instruments). Therefore, to set up a proper baseline for a given task, it is reasonable to start with the application of the simplest potentially suitable approach. The thresholding approach can be considered as a good starting point due to the following reasons: ship plumes in a simplified setting can be considered as a blob of pixels with a concentration higher than the surrounding environment; the thresholding method does not require human labeling (unsupervised learning) and could be directly applied on the data.

RQ6: *Can we improve the segmentation quality of NO_2 plumes from individual ships using supervised machine learning?*
Once the simplest baseline is established, we would like to understand how the quality of ship plume segmentation can be improved once a more complex methodology is applied. With supervised machine learning, we provide the model with the human labels of the position of the NO_2 plume of interest. With this, the model could pick up the nonlinear dependencies that differentiate a pixel that belongs to a plume from a pixel that is part of the background.

RQ7: *Does the machine learning-based segmentation allow for the detection of NO_2 plumes that cannot be recognized visually?*
The fact that some of the NO_2 plumes cannot be recognized when visually studying the data, does not mean that the signal has not been registered by TROPOMI. Among other reasons, there can be an insufficiently detailed color scheme selected when visualizing the data, or insufficient capabilities of the human eye. Such a signal could still potentially be recognized by a machine-learning model.

RQ8: *How to identify ships that are potential anomalous emitters using TROPOMI data?*
Another characteristic of the problem of ship emission monitoring is the fact that the ground truth data are not available. Potential bias of the TROPOMI measurements above the open sea on a global scale is unknown (there are no stationary in-situ measurement points). Moreover, due to the nonrigid structure of the ship plume, and the fact that some of the signal related to the plume can be below the detection capabilities of the human eye, the human-made labels used for the training of the ship-plume segmentation model may contain errors.

1.5 Outline

This thesis is based on a series of publications. The chapters present articles that have been peer-reviewed and published. The exceptions are this chapter and Chapter 2, which serve as background. Each following chapter of the thesis builds upon the findings of its predecessor, as a whole representing state-of-art knowledge in the application of TROPOMI satellite data for the monitoring of NO_2 emission from individual seagoing ships. The structure of the thesis is as follows:

In **Chapter 2**, we explain the general workflow that will be used in the thesis and introduce data sources that are necessary to combine in order to perform a ship NO_2 emission monitoring using TROPOMI data.

In **Chapter 3**, using the developed machine learning-based methodology, we examine the sensitivity limits of the detection system using TROPOMI data with respect to the detection of NO_2 plumes from individual seagoing ships. With this, we set up the research scope for further study. The chapter is based on the paper:

- Kurchaba, S., Sokolovsky, A., van Vliet, J., Verbeek, F.J., Veenman, C.J., 2024. Sensitivity analysis for the detection of NO_2 plumes from seagoing ships using TROPOMI data. Remote Sensing of Environment 304, 114041. doi:10.1016/j.rse.2024.114041.

After the limits of the satellite capabilities are established, we focus our attention on the evaluation of ship NO_2 emission. To focus the area of analysis on the region where the ship plume is expected to be located, in **Chapter 4**, we present a method that enables the automated assignation of a region of interest (RoI) to a studied ship. The RoI of a ship is established based on information about the position of the ship as well as the speed and the direction of the prevailing winds so that the plume of the studied ship is located within the designated area. Using the RoI of the ship, we can show the first attempts of automatic segmentation of a ship's plume. The chapter is based on the conference paper:

- Kurchaba, S., van Vliet, J., Meulman, J.J., Verbeek, F.J., Veenman, C.J., 2021. Improving evaluation of NO_2 emission from ships using spatial association on TROPOMI satellite data, in: 29th International Conference on Advances in Geographic Information Systems, pp. 454–457. doi:10.1145/3474717.3484213.

In **Chapter 5**, we study the possibilities of improving the quality of ship plume segmentation. To address the problem, we use supervised machine learning. Based on the previously defined RoI of a ship, we construct a set of features for training a classification model to distinguish pixels that are part of a plume of a studied ship from those that are not. The chapter is based on the paper:

- Kurchaba, S., van Vliet, J., Verbeek, F.J., Meulman, J.J., Veenman, C.J., 2022. Supervised segmentation of NO_2 plumes from individual ships using TROPOMI satellite data. Remote Sensing 14. doi:10.3390/rs14225809.

In **Chapter 6**, we focus on developing a methodology for the automated detection of anomalously emitting ships. We leverage the methodology presented in the previous chapter, combining the RoI of a ship and a supervised method of ship plume segmentation, with a proposed machine-learning-based regression model for estimating NO_2 from ships. The chapter is based on the paper:

- Kurchaba, S., van Vliet, J., Verbeek, F.J., Veenman, C.J., 2023. Anomalous NO_2 emitting ship detection with TROPOMI satellite data and machine learning. Remote Sensing of Environment 297, 113761. doi:10.1016/j.rse.2023.113761.

Lastly, in **Chapter 7**, we present the main conclusions of the dissertation and possible directions for future work.