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

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Chapter 7

Conclusions and future work

In this Chapter, we recapitulate the work presented in this thesis. We summarize the research findings that were presented in the preceding chapters and revisit the research questions outlined in the Introduction chapter. Finally, we present an overview of future research opportunities with regard to the application of the TROPOMI instrument or next-generation satellite-based instruments for the task of monitoring of NO_x emission from shipping.

In Chapter 3, we examined the sensitivity limits of TROPOMI data with respect to the detection of NO_2 plumes from individual seagoing ships. In that Chapter, we addressed three 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 the detection system using TROPOMI data?

- **RQ2:** To what extent can the detectability of NO_2 plumes be improved if only the biggest emitters are taken into account?

- **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?

We addressed the above-mentioned questions with a classification model trained to separate image patches into those with and without ship plumes. We proposed to estimate the detection capabilities of the detection system using TROPOMI data based on parameters such as speed and length of the ship, as those are known to be good estimates of ship emission potential. The study was performed for four regions of interest: the Mediterranean Sea, Arabian Sea, Biscay Bay, and Bengal Bay.

Addressing **RQ1**, we first demonstrated that the smallest ships in our dataset fall below the detection limit. However, once a certain level of ship speed/size is reached, the ship plume becomes detectable with our method. Subsequently, we calculated that for the Mediterranean Sea and the Arabian Sea, the sensitivity limits of the studied detection system are approximately $1 \times 10^7 m^5/s^3$. For the Biscay Bay, the sensitivity limit is lower and is around $3.8 \times 10^6 m^5/s^3$ (c.f. Figure 3.10). Translating this into ship speed and length, we infer that, for the Mediterranean and Arabian Seas, ships slower than 10 knots or shorter than 150 meters are below the sensitivity limit of the detection system using TROPOMI data. For the Biscay Bay, the limit lies around 8 kt and 100 m. For Bengal Bay, we were not able to estimate the sensitivity limit due to the insufficient amount of data.

With respect to **RQ2**, our results indicate that restricting the analysis to faster/larger ships leads to enhanced detectability of ship plumes. This suggests that focusing on the larger emitters could potentially increase the efficiency of the application and accuracy of ship emission monitoring using the TROPOMI instrument. The analysis also shows differences in model performance between studied regions. We concluded that these variations could be partially attributed to variations in ship traffic density between the regions. Additional factors that potentially can influence the performances of the models are measurement conditions (e.g., number of cloudy days), differences in data quality between regions, and different scales of temperature fluctuations or concentration of ozone in the background.

When addressing **RQ3**, we again encountered the variability of the results across the regions. For the Mediterranean Sea and Biscay Bay, an increase in data volume led to a notable enhancement in model performance. While, for the Arabian Sea and Bengal Bay, the impact of increasing the amount of data, even though present, was less pronounced. One of the reasons was the fact that for European regions we had a higher ratio of data points with a high value of emission proxy in the dataset than for the Bengal Bay and Arabian Sea. Nonetheless, the obtained results indicate that the accuracy of currently determined detection limits is perhaps constrained not only by the methodology or the sensor but also by data availability.

In Chapter 4, we addressed the research questions:

- **RQ4:** How to assign a TROPOMI signal associated with a certain plume to a potential emitting ship?

- **RQ5:** To what extent can the NO_2 plumes be segmented in the TROPOMI data using a simple thresholding method?

To address **RQ4**, we proposed a method for automated assignment of the region of interest (RoI) to the analyzed ship. We called the proposed RoI a *ship sector*. The *ship sector* is defined based on AIS data, information about the speed and direction of the prevailing wind, as well as assumed uncertainties in the speed and direction of the wind data. The *ship sector* is defined such that the plume produced by an analyzed ship will always be located within it. Moreover, the proposed approach provides a possibility for large-scale automatic processing of satellite data for the quantification of emissions from individual seagoing ships. Addressing **RQ5**, we concluded that ship plume segmentation within the assigned *ship sector* requires a more complex method than the linear threshold. Indeed, when comparing the estimated values of NO_2 with the ship emission proxy, we obtained low linear correlation scores, calling for a more complex methodology for ship NO_2 estimation.

Therefore, in Chapter 5, we focused on the development of a supervised machine learning methodology for ship plume segmentation within a *ship sector*. The presented methodology is based on task-specific feature engineering that allows to address ship plume segmentation with a multivariate model. Using the developed methodology, the following research questions were studied:

- **RQ6:** Can we improve the segmentation quality of NO_2 plumes from individual ships using supervised machine learning?
- **RQ7:** Does the machine learning-based segmentation allow for the detection of NO_2 plumes that cannot be recognized visually?

To address **RQ6**, we studied a list of multivariate classifiers of increasing complexity and compared them with the threshold-based benchmarks. With the best (XGBoost) model, we achieved more than 20% increase in the segmentation average precision in comparison to the best benchmark model. We can state that the application of supervised machine learning can indeed improve the quality of ship plume segmentation.

In Chapter 5, we also showed that with an XGBoost model, we can segment more plumes while achieving 6.8% higher correlation with the emission proxy than when the plumes were segmented manually. This result suggests that the machine learning-based segmentation allows for the detection of NO_2 plumes that were not recognized visually (**RQ7**).

Finally, in Chapter 6, we focused on the last research questions:

- **RQ8**: How to identify ships that are potential anomalous emitters using TROPOMI data?

To identify anomalously emitting ships, we presented a method that combines two independently trained machine-learning models. Based on the models' responses, we identify ships that emit more than can be expected based on the operating conditions and characteristics of the ship. To minimize the effects of disruptive events (weather, neighboring another ship, or land outflow), we observed each analyzed ship for an extensive period of time, creating respective ship profiles. Ships that are ranked as highly deviating throughout the time of observation according to both machine learning models, are considered to be potential anomalous emitters and require further attention. If no other explanations can be found, the ships are advised to be the candidates for inspection.

7.1 Future directions

Referring back to the overarching research question of the thesis, we can state that indeed the TROPOMI instrument has the potential to be used for monitoring NO_2 emissions from individual ships on a global scale. Nevertheless, to make such an application industrially operational, several challenges still need to be addressed:

- Attribution of a signal to individual ships in case of overlapping plumes. In this thesis, we reduce this issue by means of the application of multi-day data averaging. This is suitable when drawing conclusions on the basis of long-term observations. However, in order to observe day-to-day changes in the level of emissions produced by a ship, the solution should be adapted.

- The study of other chemical compounds that can be used by machine-learning models as an additional signal of ship plumes. Throughout the thesis, we witnessed that NO_2 plumes from such comparable sources of emissions as ships are often difficult to detect in TROPOMI signals. However, it is known from the literature that the presence of gases such as ozone (O_3) or formaldehyde (HCHO) may be coupled with the presence of ship plumes [27, 44, 53, 2]. The current quality of satellite-based measurements does not allow to distinguish ship traces of these components on daily data. Yet, multi-day averaging confirms that the HCHO signal from ships is present in the data [72, 44], while the concentration of O_3 in the background affects the speed of $NO_x \longrightarrow NO_2$ transformation [19].

- The investigation of causes for regional differences observed in TROPOMI sensitivity with respect to the detection of NO_2 plumes from individual ships. In Chapter 3, we showed that the sensitivity limits of the instrument vary significantly depending on the region under study. We see that it can be explained partially by the traffic density in the region. However, we do not have evidence to state that the latter is the only cause of the differences observed. Other potential sources of regional differences can be varying ozone concentrations, wind speed, or the presence of emitters that are not registered with AIS (e.g. oil rigs or military ships).

We believe that by tackling the aforementioned directions, we can improve the overall understanding of the potential of the application of the TROPOMI instrument with respect to ship emission monitoring.

7.2 Final remarks

Summarizing our conclusions, we can state that with the work presented in this thesis, we notably moved forward the state-of-the-art with respect to the application of satellite observations for the task of continuous and global monitoring of emissions from individual ships. When starting the work of this thesis, all we knew was that some of the plumes from individual ships could be distinguished with the TROPOMI instrument. When reaching the end, we know the sensitivity limits of the detection system of ship NO_2 plumes using TROPOMI data, how to process the TROPOMI signal to extract information about the ship emissions automatically, and how to automatically select ships that are potential anomalous emitters.

The aim of this thesis has been to improve the quality of monitoring of emissions coming from the shipping industry, toward mitigating its adverse environmental effects. A collaborative and continuous effort of professionals across various domains and fields of expertise is essential to ensure that both monitoring of ship emissions and related policies yield the intended outcomes. Indeed, it was noted recently that the implementation of the nitrogen emission control area (NECA) in the North and Baltic Seas in 2021 had little impact on remotely measured NO_x concentrations in European waters [104]. The work presented here is just a piece of a complicated web of required actions, reactions, and decisions necessary to achieve desired environmental outcomes. Nonetheless, we believe that it lays a solid foundation for the future applications of satellite observations for the monitoring of emissions (including but not limited to NO_2) produced by individual ships. In this manner, it will contribute to mitigating the environmental impact of the shipping industry as a whole.