

**23rd International Conference on
Harmonisation within Atmospheric Dispersion Modelling
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Harmonizing Machine Learning and Numerical Dispersion Modelling for Improved Ship Emission Source Identification

Guanzhong Wang, Institute for Applied Physics and Measurement Science, University of the Bundeswehr Munich, Neubiberg, Germany, guanzhong.wang@unibw.de

Ronny Badeke, Hereon Institute of Coastal Environmental Chemistry, Helmholtz-Zentrum Hereon, Geesthacht, Germany

Heinrich Ruser, Institute for Applied Physics and Measurement Science, University of the Bundeswehr Munich, Neubiberg, Germany

Julian, Schade, Institute of Chemistry and Environmental Engineering, University of the Bundeswehr Munich, Neubiberg, Germany

Thomas Adam, Institute of Chemistry and Environmental Engineering, University of the Bundeswehr Munich, Neubiberg, Germany

Abstract

Monitoring emissions from the fuel combustion of seagoing ships is a prerequisite for assessing their harmful impacts and for seamlessly checking whether local regulations are complied with. We present results from a measurement campaign in Darsser Ort on the south coast of the Baltic Sea, approx. 20 – 40 km east of the main shipping routes and approx. 40 km north-east of the port of Rostock (Germany), the largest freight and passenger port in the area. During the two-month-long campaign the chemical composition of about 1.6 million individual aerosol particles was analyzed using single-particle mass spectrometry (SPMS). We developed a deep learning model to automatically classify the SPMS data according to characteristic ion combinations in the bipolar mass spectra, in order to analyze ship fuel emissions in real time. Combined with local wind data (speed and direction) and Automatic Identification System (AIS) ship identification and position data, ships operating on polluting types of fuel could be identified and localized. We verified our findings on back-traced ship engine emissions by simulating exhaust plume distributions using a sophisticated aerosol transport model (EPISODE-CityChem). In many cases, the model chain successfully replicates emission events detected by chemical profiling of individual aerosol particles with matching temporal detail. In particular, correlating the results of both approaches leads to robust and reliable assignment of detected emissions to specific ships.

Introduction

Ships are essential to global trade, transporting over 80% of the world's goods, and this number is expected to increase (UNCTAD, 2023). At the same time, maritime transportation contributes significantly to air pollution and poses serious health risks for inhabitants living along major shipping routes (Eyring et al., 2010). The International

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Maritime Organization (IMO) has established Sulfur Emission Control Areas (SECA, including the Baltic Sea, the North Sea, most of the US and Canadian coasts, etc.) requiring ships to use low-sulfur fuels ($\leq 0.1\%$ sulfur) or to install exhaust gas cleaning systems (e.g., scrubbers) if high-sulfur fuels like heavy fuel oils (HFO) are still used. Consequently, there is an urgent need for effective monitoring. Most ship emission monitoring systems rely on gas-phase instruments to measure changes in gas concentrations such as CO_2 , SO_x , and NO_x . However, since gases are rapidly diluted, the effectiveness of such systems is limited to distances of a few hundred meters only (Zhou et al., 2022). The coverage of the monitoring system can be effectively extended by using particle-phase measurements, as aerosol particles retain the chemical composition associated with their sources even after long-distance transport (Dall'Osto and Harrison, 2006).

Single-particle mass spectrometry (SPMS) is a mature, real-time technique to quantify the chemical composition of individual aerosol particles. It is capable of analyzing hundreds of particles per minute by laser desorption/ionization (LDI). To handle this large volume of data, machine learning methods are increasingly used for rapid and accurate classification of SPMS data (Wang et al., 2024a, 2024b).

In this study, our focus is on detecting aerosol particles from ship emissions, especially those resulting from polluting HFO combustion. To accurately identify and localize HFO-emitting ships, the method integrates three components: (1) convolutional neural networks (CNN)-based particle classification, (2) local wind data (direction and speed), and (3) ship trajectory data from the Automatic Identification System (AIS). In our previous research, we have explored data with monitoring ranges of up to 2 km (Wang et al., 2025). This time the goal is to achieve long monitoring ranges of up to 40 km from the emission source. We implemented simulations using a chemistry transport model (EPISODE-CityChem) to validate the recognition of remote emission sources.

Measurement Campaign and Data Analysis

Data were obtained during a measurement campaign at the northernmost point of the Darss Peninsula on the German coast of the Baltic Sea. The Sampling Site ($54^\circ 28' 28.4''\text{N}$, $12^\circ 30' 13.9''\text{E}$) was located approximately 20 to 40 km east of the main shipping routes and around 40 km northeast of Rostock, the largest port in the region (see Figure 1). Between May 11 and July 19, 2023, approximately 1.6 million individual aerosol particles were analyzed using SPMS. The SPMS's operating principle has been described in detail elsewhere (Passig and Zimmermann, 2021).

Figure 2 shows several examples of chemical signatures from particles originating from different sources. The mass spectrum (MS) is discretized with a mass-to-charge (m/z) interval of 1. The spectra cover an m/z range from -120 to $+120$ and are normalized to the maximum intensity within the positive and negative spectra, respectively. In general,

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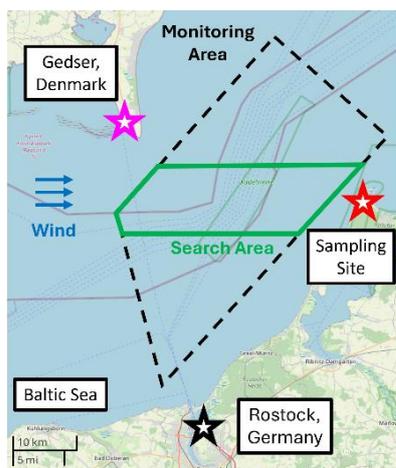


Figure 1: Map of the monitoring area and the main shipping routes

the classes can be assigned based on the main ion markers in the mass spectrum. The objective of this study is to identify V-rich particles in the atmosphere from the combustion of HFO (i.e., abundance of $^{51}\text{V}^+$, $^{67}[\text{VO}]^+$; $^{54/56}\text{Fe}^+$; $^{58/60}\text{Ni}^+$ ions, see Figure 2(e)).

We designed a CNN model for the classification of SPMS data, which achieved a classification accuracy of $\sim 93\%$ for the 13 classes of particles. For more details on the model architecture and the training process, see Wang et al. (2024b).

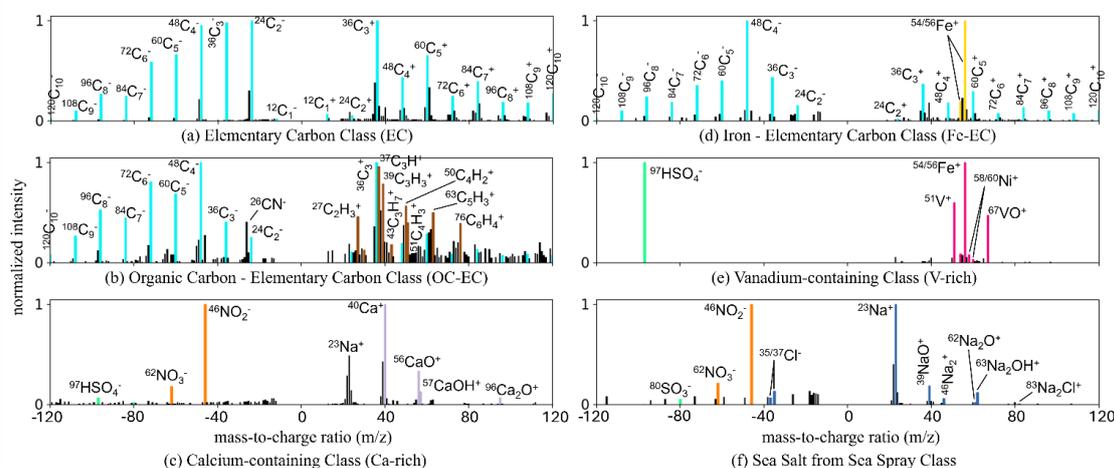


Figure 2: Examples of mass spectral patterns for 6 classes of aerosol particles

Results and Discussion

Based on the defined Monitoring Area, a Search Area is generated (see Figure 1) in accordance with the wind direction recorded at the local weather station (German Weather Service (DWD) Station ID 6097). Figure 3(a) shows the wind data for one day (May 24, 2023). The aerosol particles analyzed by SPMS were classified by the trained CNN model in real time. Figure 3(b) illustrates the classification results for the same day. Exemplarily, between 18:00 and 18:40, up to 40% of all detected particles were assigned to the V-rich class. Using the time interval T_{Detect} of this event, the distances from the boundaries of the Search Area to the Sampling Site are calculated, as well as the time interval T_{Travel} it takes for particles to reach the Sampling Site, considering the actual wind direction and speed. $T_{\text{Search}} = T_{\text{Detect}} - T_{\text{Travel}}$ is then the time interval when ships emitting V-rich particles traveled in the Search Area. To identify these ships, the AIS database is searched for entries that appeared during T_{Search} within the Search Area.

With this method, ships responsible for significant emissions of V-rich particles — and therefore suspected of using HFO — can be swiftly localized by calculations based on wind speed, wind direction and AIS. To further strengthen and confirm source attribution,

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we additionally applied urban-scale numerical modelling based on the EPISODE-CityChem model, utilizing the Moving Point Source (MPS) algorithm to simulate the dispersion of moving exhaust plumes (Badeke et al., 2024; Karl et al., 2019). Table 1 shows the results of combined calculations and simulations for the localization of seven ships with significant emission of V-rich particles during the particular event (18:00-18:40). For four of these seven ships, the localization derived from local wind parameters was confirmed since it coincides with the back-traced simulated emission plume dispersion, i.e. the arrival time interval of the simulated plumes was also between 18:00 and 18:40. Figure 4 shows two simulation results as examples.

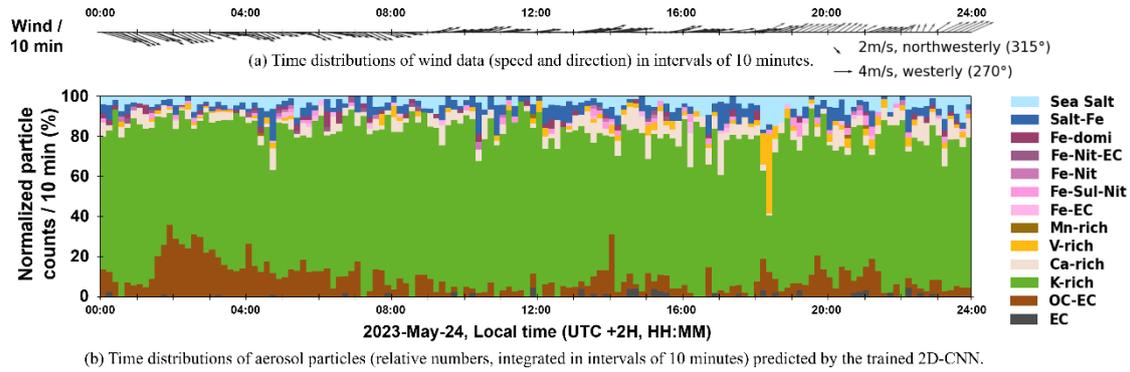


Figure 3: Exemplary results for 24 hours of measurements (May 24th, 2023) at Darsser Ort. (a) Wind speed and direction from the local DWD weather station, displayed in intervals of 10 minutes, with scales of speed and direction (angle) given on the right. (b) Time distribution of aerosol particle classes predicted by the trained CNN model, with relative numbers of particles per class, integrated in intervals of 10 minutes.

Table 1: Search model identification results validated with plume dispersion simulations for ships associated with the V-rich event detected in the time interval 18:00-18:40. The actual wind speed and direction were (5.7 ± 0.2) m/s and $(266 \pm 5)^\circ$ (west wind). Directions of travel of ships are marked as N-north, E-east, S-south, W-west.

Ship confirmed by search model	Type of ship	Length of ship	Min. distance to meas. site	Direction of travel	Dispersion simulation of plumes arrival time
SHIP1	Passenger	170 m	36 km	S→N	Max. plumes arrived at 17:20
SHIP2	Passenger	219 m	20 km	E→W	Confirmed
SHIP3	Cargo	158 m	25 km	E→W	Confirmed
SHIP4	Tanker	274 m	25 km	E→W	Max. plumes arrived at 20:00
SHIP5	Tanker	183 m	20 km	E→W	Max. plumes arrived at 17:10
SHIP6	Cargo	163 m	20 km	E→W	Confirmed
SHIP7	Tanker	250 m	18 km	W→E	Confirmed

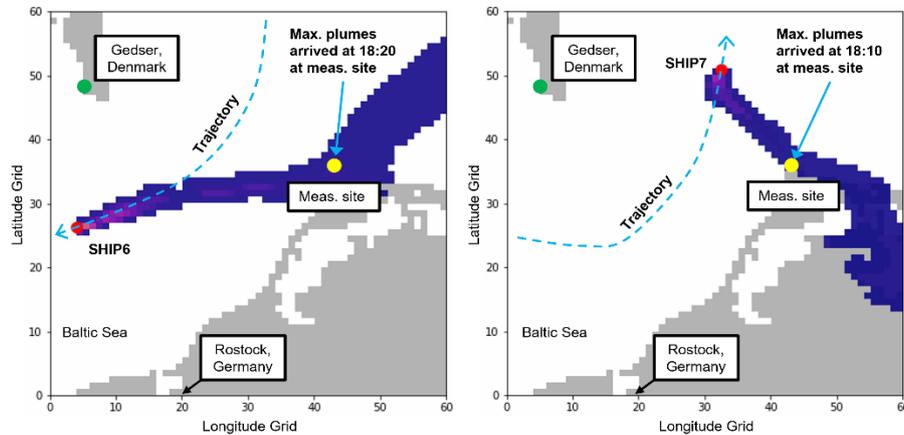


Figure 4: EPISODE-CityChem simulation results utilizing the MPS algorithm for SHIP6 and SHIP7

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Conclusion

The integrated system enables real-time detection of ships burning heavy fuel oil (HFO). Ambient aerosols are continuously sampled, chemically profiled, and automatically classified using deep learning. By integrating these classifications with meteorological data and AIS ship information, the system achieves real-time localization of ships using HFO. Cross-comparison of the identified emission events with simulation outputs for plume dispersion further enhances the reliability of source attribution to specific ships. While not as complex as full dispersion models, the search model approach offers a practical and efficient real-time solution, particularly in cases where inverse simulations from measurement data are not feasible.

Acknowledgements

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References

- Badeke, R., Matthias, V., Sankaran, A., Kähler, C., Schade, J., Jeong, S., and Adam, T., 2024. Integrating wind tunnel, numerical model and measurement data for ship plume assignment, PHYSMOD conference, Lyon.
- Dall’Osto, M., Harrison, R., 2006. Chemical characterisation of single airborne particles in Athens (Greece) by ATOFMS. *Atmospheric Environment* 40, 7614–7631. <https://doi.org/10.1016/j.atmosenv.2006.06.053>
- Eyring, V., Isaksen, I.S.A., Berntsen, T., Collins, W.J., Corbett, J.J., Endresen, O., Grainger, R.G., Moldanova, J., Schlager, H., Stevenson, D.S., 2010. Transport impacts on atmosphere and climate: Shipping. *Atmospheric Environment, Transport Impacts on Atmosphere and Climate: The ATTICA Assessment Report 44*, 4735–4771. <https://doi.org/10.1016/j.atmosenv.2009.04.059>
- Karl, M., Walker, S.-E., Solberg, S., Ramacher, M.O.P., 2019. The Eulerian urban dispersion model EPISODE – Part 2: Extensions to the source dispersion and photochemistry for EPISODE–CityChem v1.2 and its application to the city of Hamburg. *Geoscientific Model Development* 12, 3357–3399. <https://doi.org/10.5194/gmd-12-3357-2019>
- Passig, J., Zimmermann, R., 2021. Laser Ionization in Single-Particle Mass Spectrometry, in: Zimmermann, R., Hanley, L. (Eds.), *Photoionization and Photo-Induced Processes in Mass Spectrometry*. Wiley, pp. 359–411. <https://doi.org/10.1002/9783527682201.ch11>
- UNCTAD, 2023. Review of Maritime Transport 2023: Towards a Green and Just Transition. United Nations. <https://doi.org/10.18356/9789213584569>
- Wang, G., Ruser, H., Schade, J., Jeong, S., Passig, J., Zimmermann, R., Dollinger, G., Adam, T., 2025. Deep learning based aerosol particle classification for the detection of ship emissions. *Science of The Total Environment* 994, 180041. <https://doi.org/10.1016/j.scitotenv.2025.180041>
- Wang, G., Ruser, H., Schade, J., Passig, J., Adam, T., Dollinger, G., Zimmermann, R., 2024a. Machine learning approaches for automatic classification of single-particle mass spectrometry data. *Atmospheric Measurement Techniques* 17, 299–313. <https://doi.org/10.5194/amt-17-299-2024>
- Wang, G., Ruser, H., Schade, J., Passig, J., Zimmermann, R., Dollinger, G., Adam, T., 2024b. CNN-Based Aerosol Particle Classification Using 2D Representations of Single-Particle Mass Spectrometer Data, in: *2024 International Conference on Artificial Intelligence in Information and Communication (ICAIIIC)*, pp. 1–6. <https://doi.org/10.1109/ICAIIIC60209.2024.10463253>
- Zhou, F., Fan, Y., Zou, J., An, B., 2022. Ship emission monitoring sensor web for research and application. *Ocean Engineering* 249, 110980. <https://doi.org/10.1016/j.oceaneng.2022.110980>