

The detection of Benzene, Toluene, and Xylenes (BTX) in water is critical for assessing pollution in aquatic environments, as these compounds pose significant environmental and public health risks. Traditional methods for BTX monitoring often require lab-based analysis, causing delays in obtaining actionable data. This study introduces an innovative use of portable Membrane Inlet Mass Spectrometry (MIMS) for the rapid, on-site detection of BTX. It provides a swift, efficient, and dependable method for real-time monitoring of environmental contaminants in waterways, particularly in the wake of natural catastrophes where immediate assessment of water quality is essential for mitigating further environmental damage and protecting public health.

Introduction



As environmental challenges intensify due to both natural disasters and human activities, pollution has become a major global issue. The contamination of natural resources—especially water, air, and soil—by harmful chemicals poses severe risks to biodiversity and public health, while also disrupting ecological balance. Rapid detection and mitigation of pollutants are essential, particularly in scenarios such as industrial accidents or environmental catastrophes, where time is of the essence to prevent further harm.

Catastrophic events, including extreme weather and water-related phenomena such as storm surges, floods, and droughts, can severely impact water quality by introducing hazardous pollutants into aquatic systems. These extreme conditions often lead to sudden and extensive contamination, heightening the need for rapid detection methods like Membrane inlet mass spectrometry (MIMS).



Portable MIMS technology offers:

- mitigate the environmental and public health risks associated natural disasters, preventing long-term damage to ecosystems and water resources
- offers a cutting-edge approach to environmental monitoring, specifically for the assessment of water quality.
- enables the real-time detection of volatile organic compounds (VOCs) and other pollutants directly at the source, without the need for labor-intensive laboratory-based sample preparation. This in-situ monitoring capability allows for immediate and accurate analysis,



Motivation and concept

This research aims to validate a portable Membrane Inlet Mass Spectrometry system for in-field analysis of Benzene, Toluene, and Xylenes in river canal water. By utilizing a quadrupole mass spectrometer with a polydimethylsiloxane (PDMS) membrane inlet, the study examines the system's efficiency in detecting BTX both in controlled laboratory conditions and real-world samples from the Danube–Tisa–Danube (DTD) canal.

Table 1 List of the BTX compounds used for validation of the MIMS method.

Compound	CAS number	Molecular weight (g/mol ⁻¹)	Target Ion (m/z)	MRL (I, II class of water) µg L ⁻¹	MRL (drinking water) µg L ⁻¹
Benzene	71-43-2	78.11	78, 77	500	2
Toluene	108-88-3	92.14	91, 92	500	700
Xylene	1330-20-7	106.168	105, 106	50	50

The details of the compounds of interest are presented in Table 1, including their molecular weights, target ions, and maximum residue levels (MRLs) allowed in drinking and irrigation water. The MRL limits are expressed in micrograms per litre of water (mgL⁻¹) as determined by the regulations of the Republic of Serbia where class I and II can be used for irrigation.

Our testing, calibration, and validation of the MIMS portable analytical system for water-quality monitoring were carried out in accordance with the relevant guidance documents. Following the guidelines for the validation and verification of quantitative and qualitative test methods and the analytical quality control requirements, we clearly demonstrate that BTX from water can be successfully quantified with a high level of confidence in the results.

Experimental set up

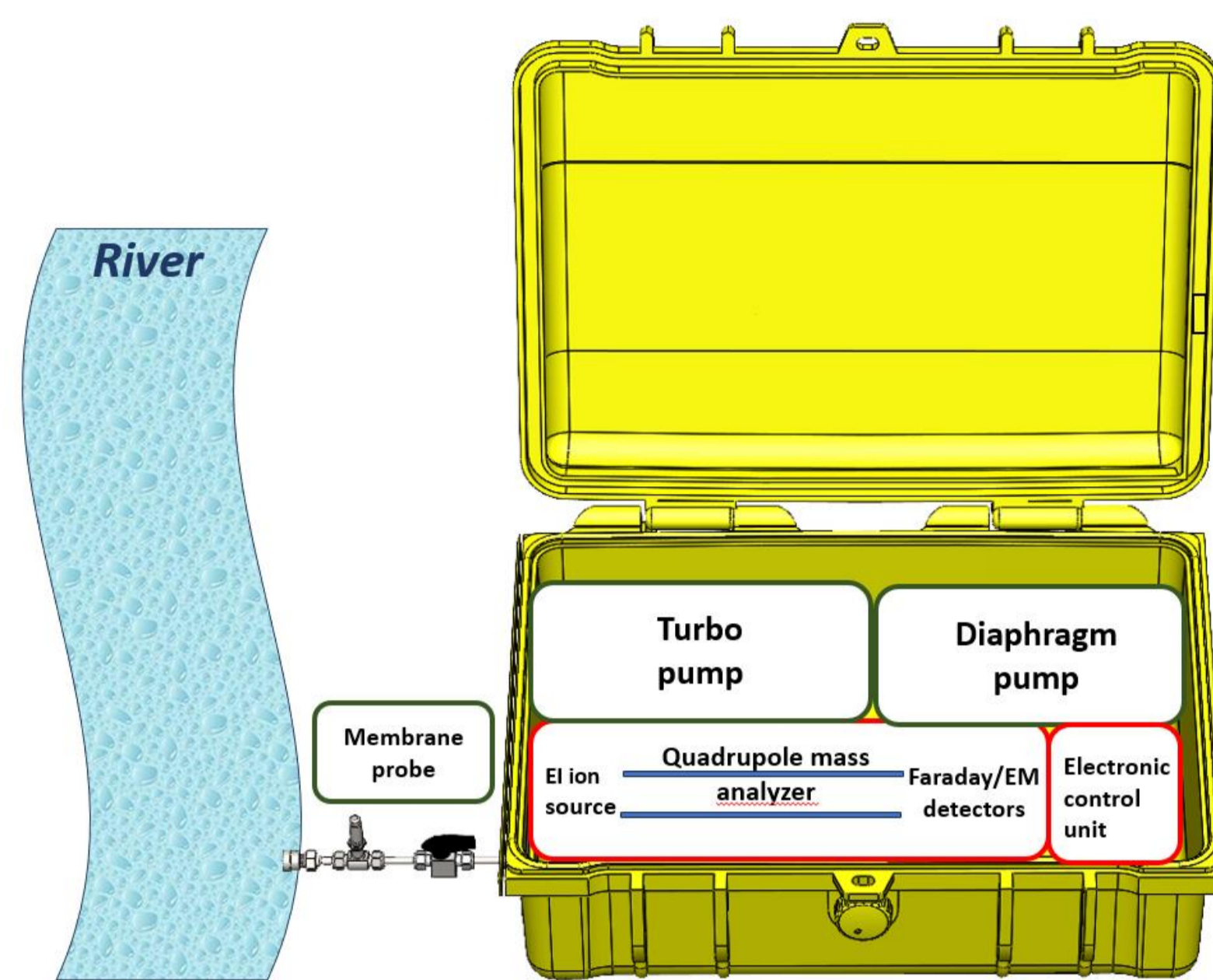


Fig. 1 Schematic of the MIMS system used for the river canal water monitoring

The experimental setup utilized MIMS system (Fig. 1) designed for real-time monitoring of organic contaminants in water. The system employed a PDMS membrane inlet, which selectively allowed organic compounds to pass through while blocking water. This facilitated the separation and detection of analytes using a quadrupole mass spectrometer with a mass range of 1–300 amu. The vacuum system consisted of a diaphragm pump and a turbomolecular pump, ionization was achieved through an open electron impact (EI) ion source with yttriated iridium filaments. The MIMS system was compact, with dimensions of 25 cm x 50 cm x 60 cm and a weight of 25 kg, making it suitable for field applications and real-time analysis of water samples.

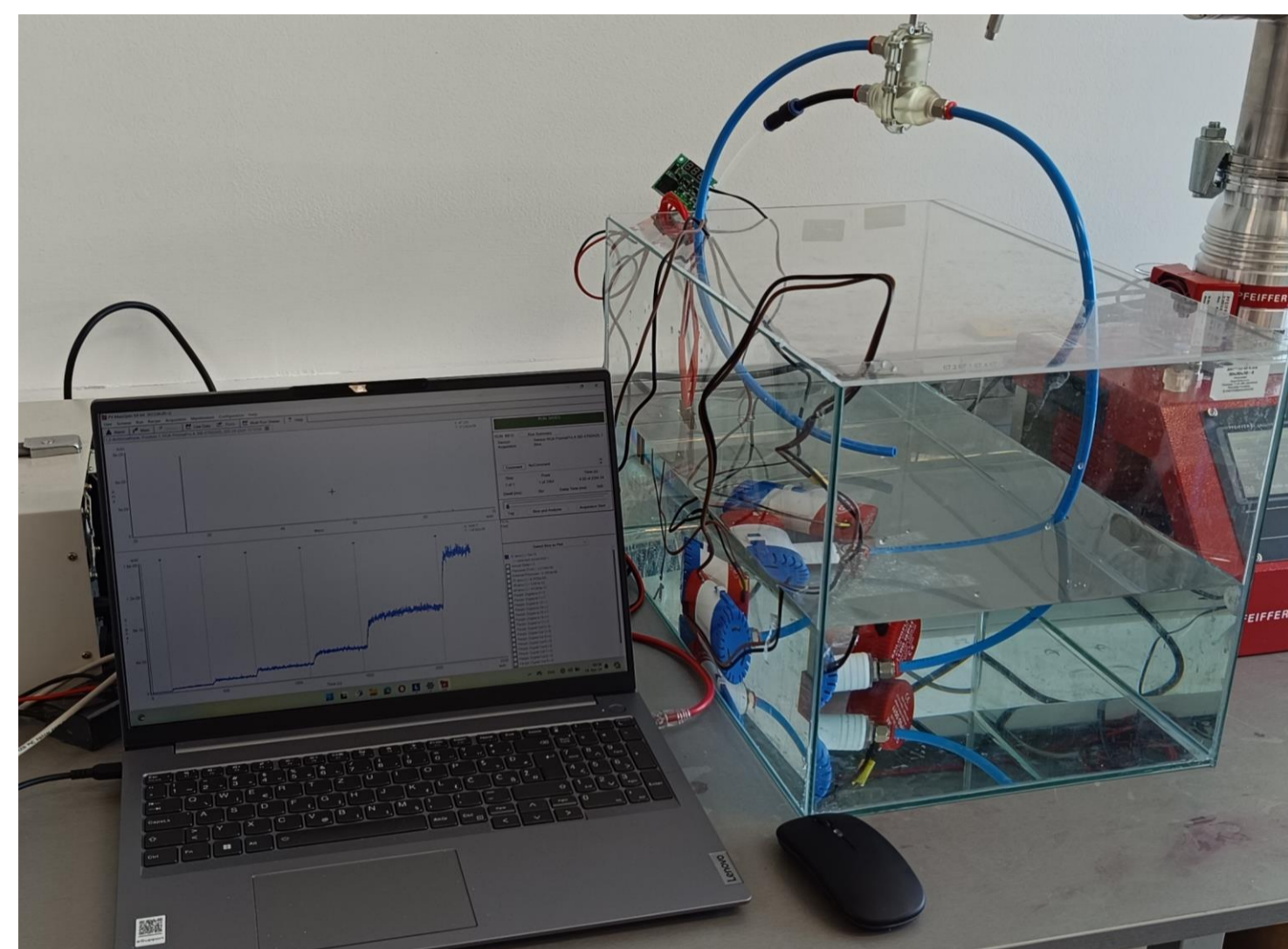


Fig. 2. Temperature-controlled aquarium with continuous mixing used for sample preparation.

A water analysis method was developed based on oil-in-water monitoring technique. During field tests on river canal water, a membrane sample probe was connected to the water flow system via a PA hose. The method was compared with a lab technique for quantifying BTX residues in water. Validation used DI water and DTD canal water, spiked with BTX standards at concentrations from 10 to 250 mg/L. Samples were prepared in a temperature-controlled aquarium with continuous mixing, and the membrane probe was inserted directly for analysis (Fig 2.). All measurements were taken at ambient temperature. The sample was introduced directly into the vacuum system.

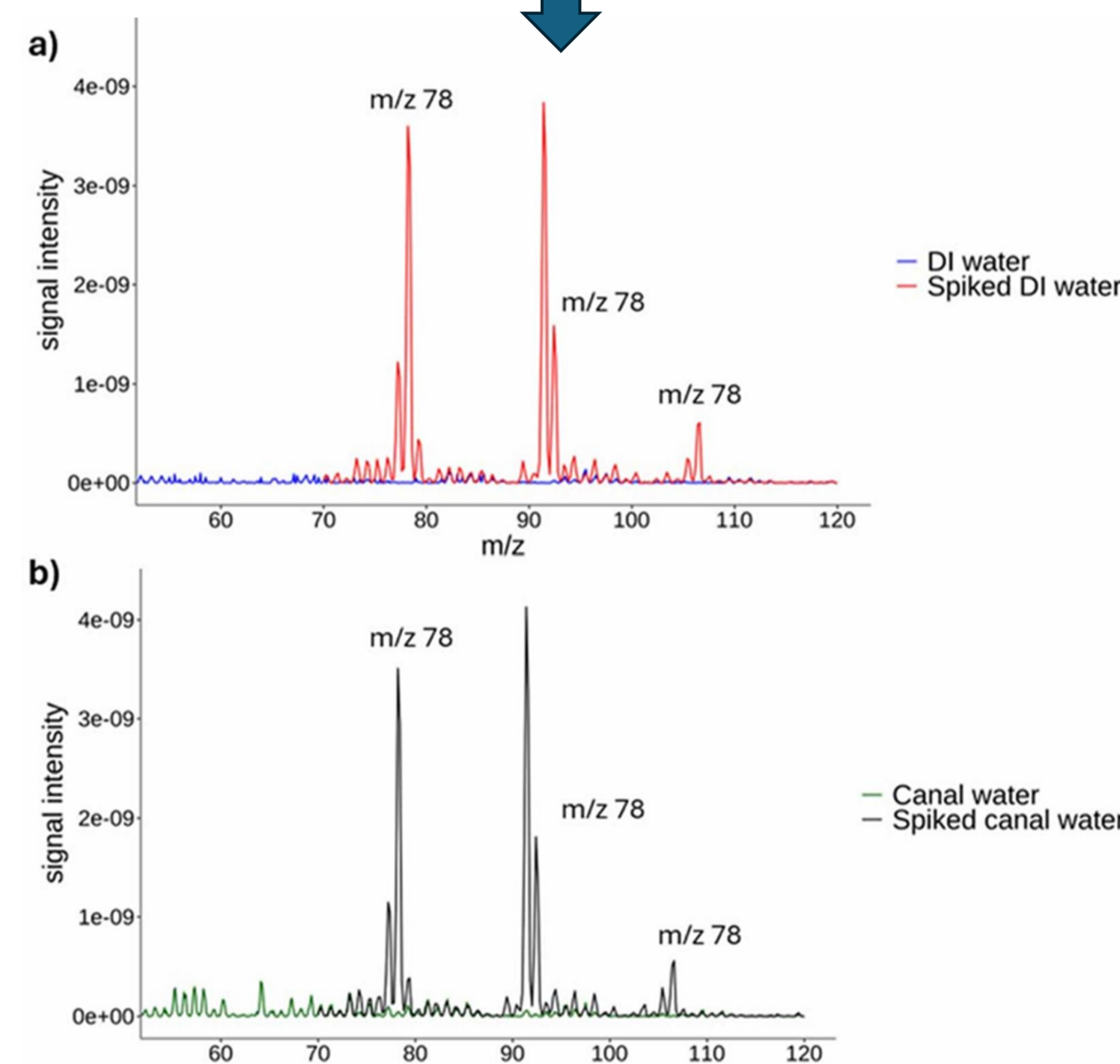


Fig. 3. Full scan of pure and spiked samples for (a) DI water and (b) canal water using the portable MIMS.

The analysis of BTX in water and the total time needed for the on-site analysis was ~10 min. During the validation study, all the tests were performed in the analytical range from 10–250 mgL⁻¹ to confirm the linearity, specificity, selectivity, accuracy, and precision of the method, and to determine the detection and quantification limits.

Developed analytical method was able to distinguish the analyte(s) of interest from endogenous components in the matrix or other components in the sample, without interference. Fig. 3 a) displays the selectivity of the method when using DI water, while Fig. 3 b) illustrates the influence of the matrix on the selectivity of the method. After recording and enriching the canal water, it was observed that the selectivity of the method was at the same level as the DI water.

Table 2. Results for the LOQ and LOD values obtained using the MIMS.

Analyte	MIMS (LOD), µg L ⁻¹	MIMS (LOQ), µg L ⁻¹
Benzene	4.88	16.27
Toluene	7.43	24.77
Xylene	7.46	24.85

Limit of detection (LOD) and limit of quantification (LOQ) – for target compounds, using the MIMS, analytical standard of 10 mgL⁻¹ was used, which was added to the water sample at a defined concentrate on range. Our results show that the LOQ values were significantly lower than the MRL values for irrigation water and slightly above the MRL values for drinking water.

Conclusion

In this study, we developed and validated a portable MIMS method for the rapid, quantitative analysis of BTX in river and DTD irrigation canal water within a defined analytical range. The device's portability, fast response, and precision make it an effective tool for environmental monitoring and real-time detection of water contaminants. Its strengths include high sensitivity, quick data generation, and field usability. With advancements in MIMS technology, the system can now detect low-concentration pollutants and emerging contaminants, enhancing its utility in environmental monitoring. This makes MIMS particularly valuable in the context of natural disasters, where immediate assessment of water quality is crucial for guiding timely interventions and supporting recovery efforts.

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