

Development and optimization of the automation of Volatile Organic Compounds data analysis using an on-line TD-GC-FID/MS dual detection in the Rambouillet Forest during the ACROSS 2022 campaign

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Rambouillet Forest is a large forested location, situated about 50km from central Paris. Its size and proximity towards the capital makes it an interesting site to study the interaction between polluted air masses and biogenic emissions and the impact on air quality in areas surrounding polluted cities. The ACROSS (Atmospheric ChemistRy Of the Suburban forest) campaign represents a large international collaboration between various French, European and American institutes, which aims to further characterize these interactions. For our contribution, an on-line Thermal-Desorption Gas Chromatograph was deployed. This system is composed of two different TD-GC equipped with two Flame Ionization Detector (FID) and selectively coupled in parallel with a Mass spectrometer (MS). Each GC is designed with its own specific analytical conditions, one for light non-polar compounds and the other for monitoring heavier VOCs. During this campaign, it was the second GC that was connected to the Mass Spectrometer, to allow the identification of potential coeluted compounds. This instrument was calibrated, the complementarity between both detectors was evaluated and the system was characterized under field conditions. In general, data coverage was high throughout the campaign and as it lasted 2 months, a significant amount of data was generated. However, as data analysis can be time consuming, there is a need to improve its automation. We therefore developed an algorithm to select the most accurate result between FID and MS detection for each compound identified. This algorithm was optimized taking into account the detection limit and accuracy of each detector and the data generated during the campaign were used evaluate its efficiency at trace level concentrations.