MIGRATEWS2016-22

GAS-SOLID SURFACE MICRO SEPARATORS - VOCS TRAPPING

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KEY WORDS

BTEX detection, adsorption / desorption, kinetic theory, DSMC

ABSTRACT

The topic of the MIGRATE- ESR 10 position is “Gas-Solid Surface Micro Separators - VOCs Trapping”. The main goal of this project is to develop an analytical microfluidic method able to adsorb benzene and its derivatives and to desorb them quantitatively and rapidly by heating.

The project is offered at University of Thessaly (UTH) and In'Air Solutions (INR) with short stays in Aix Marseille University (AMU) and ICPEES. According to the time schedule the first 15 months of project will be focused on theoretical and computational kinetic theory and the DSMC method at UTH. A systematic study of the adsorption/desorption processes will be also performed. The second stay will be at AMU for 4 months working on either Navier-Stokes solvers simulating diffusion processes based on the StarCCM+ CFD s/w or in measurements of mass flow rates in microchannel. The third stay at INR will take 12 months to support the development of a microfluidic analytical device devoted to BTEX (benzene, toluene, ethylbenzene, and xylenes) measurements in air at sub ppb levels. It will include mainly experimental work aiming at improving the analytical performances of the existing analyzer such as its sensitivity by adding a preconcentration step. Based on the work conducted in UTH, as well as on updated simulations this work will aim at testing both adsorption and desorption efficiencies depending on the experimental conditions, i.e. gaseous BTEX concentrations, BTEX flow rate, residential time in the preconcentrator for adsorption or final temperature and temperature increasing for desorption. The 5 remaining months will be in ICPEES to evaluate the instrument in terms of limits of detection and quantitation, repeatability and reproducibility by using controlled gaseous BTEX concentrations in the range 0-50 ppb.

Developing ultra-portable, accurate and powerful analytical tools capable of monitoring the air pollutants in near real time has been always a challenge. As benzene has high carcinogenic effect, it is believed that it is the most harmful pollutant among all. French recommendations aim at limiting benzene concentrations in public buildings to 5 $\mu g\ m^{-3}$ (1.59 ppb) by 2018 and 2 $\mu g\ m^{-3}$ (0.64 ppb) by 2022, helping to promote the development of new highly portable instruments. ICPEES and INR recently reported the development and the optimization of a novel patented portable micro-GC based on photoionisation detection able to detect BTEX at ppb level [1]. The device is very portable (4 kg) with a very low consumption of carrier gas, less than 3.0 mL min^{-1}. This new device operates according to two consecutive steps, sampling and analysis. The system is standalone, fully controlled by homemade

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software and exhibits a time resolution of 10 minutes. The compact is highly portable and low consumable.

Based on the assessment performed by ICPEES/INR, micro-GC was tested during a field campaign aiming at highlighting the temporal variations of various pollutants concentrations inside a newly built junior high school that follows the French thermal regulation of 2005 under the MERMAID project. This experiment has shown the micro-device is able to detect every variation of toluene concentration between 2 and 18 ppb in all tested conditions which makes it perfectly appropriated for indoor air monitoring over a long period [2]. However, its current sensitivity does not permit to monitor atmospheric benzene or toluene concentration below 1 or 2 ppb.

In this regard, through numerical simulations may support a survey to develop the device performance. Under the special condition of low gas density, the discrete particle effect becomes remarkable, and discrete modeling at the meso or micro scales i.e., by implementing molecular gas dynamics or kinetic theory modeling, is required [3]. Numerical simulation of the adsorption and desorption processes are one of the challenges in this project and different models like Langmuir isotherm [4] and Brunauer-Emmett-Teller [5] will be studied. To aim this it is necessary to implement the UTH in-house deterministic and stochastic codes to couple the adsorption/desorption processes with gas-surface interaction and surface kinetics [6]. Modeling will include single gases and gas mixtures. All necessary modifications and adjustments in the UTH in-house codes will be applied to meet the specific geometry, flow and boundary conditions to perform suitable simulations obtaining reliable results to be used in the experimental part of the work.

Acknowledgements

This project has received funding from the European Union's Framework Program for Research and Innovation Horizon 2020 (2014-2020) under the Marie Skłodowska-Curie Grant Agreement No. 643095.

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