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DEVELOPMENT OF INEXPENSIVE MODULATOR FOR GCxGC-MS

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Comprehensive two-dimensional gas chromatography (GCxGC) combines high peak capacity, selectivity, resolution and efficiency in terms of number of peaks per time. Application field covers food, oils, environmental and forensic samples analysis to qualify and quantify volatile (VOCs) and semi-volatile organic compounds (SVOCs). Nevertheless, this technique is not widely used, mainly because of the high cost of pre-built GCxGC systems and separate modulators for an upgrade of existing GCs. The goal of this work was to develop an inexpensive two-step GCxGC modulator with the cost of consumables under $2000.

Agilent 7890A/5975C GC-MS was modified to GCxGC-MS. Duralumin modulator body with six ports (2 hot jets, 2 cold jets and column in/out) was built in the metal workshop for 300 USD and installed on the left inner wall of GC oven. The body of modulator was insulated from the GC oven using additional stainless steel case. The pair of cryogenic solenoid valves was installed between pressurized (1.5 bar) liquid nitrogen storage dewar and left side of the modulator. Liquid nitrogen was supplied to the valves via two 1/4" stainless steel tubes. Flow of LN2 supplied to valves was controlled using two Swagelok ball valves. For additional cooling of tubes between modulator and valves, 1/8" copper tube with flowing liquid nitrogen was wrapped around these supply tubes as previously proposed by Mostafa and Gorecki [1]. For heating purposes, the pair of two solenoid valves was installed between air compressor and front side of the modulator. For heating of supplied air, 240 V, 130 W rope heater was coiled around two 1/8" copper tubes entering GC oven from the top. It was insulated using high-temperature glass cloth. All valves were controlled by Arduino Uno microcontroller via two two-channel DC solid-state relays. Temperature of hot air supplied to the modulator was controlled by REX C-100 temperature PID controller with two K-type Omega thermocouples connected differentially [1] and located in GC oven and inside the insulation of hot air supply tubes to the modulator. Rope heater was connected via a solid-state relay. Gasoline sample was successfully analyzed using the built modulator. For quick data processing, MSD ChemStation can be used, however it lacks contour plots and other features of commercial software. To add 3D visualization, simple software was developed during one week using Python 2.7. The software works with CDF (AIA) files, it can visualize total and extracted ion contour plots, show mass spectrum at any point of the contour plot and perform NIST search. The total cost of consumables was below 1500 USD. Most of them were purchased online via Ebay, Amazon, Omega and Asco. Thus, such a modulator is very affordable and can be built in any lab.

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[1] Mostafa A, Gorecki T (2016) Anal Chem 88:5414–5423. http://dx.doi.org/10.1021/acs.analchem.6b00767