Automation of fizzy extraction enabled by inexpensive open-source modules

Hao-Chun Yang [a,b], Chun-Ming Chang [a,b], Pawel L. Urban [a,c,*]

[a] Department of Chemistry, National Tsing Hua University, 101, Section 2, Kuang-Fu Rd., Hsinchu, 30013, Taiwan
[b] Department of Applied Chemistry, National Chiao Tung University, 1001 University Rd., Hsinchu, 300, Taiwan
[c] Frontier Research Center on Fundamental and Applied Sciences of Matters, National Tsing Hua University, 101, Section 2, Kuang-Fu Rd., Hsinchu, 30013, Taiwan

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ABSTRACT

The implementation of most instrumental analysis methods requires a considerable amount of human effort at every step, including sample preparation, detection, and data processing. Automated analytical workflows decrease the amount of required work. However, commercial automated platforms are mainly available for well-established sample processing methods. In contrast, newly developed prototypes of analytical instruments are often operated manually, what limits their performance and decreases the chance of their adoption by the broader community. Open-source electronic modules facilitate the prototyping of complex analytical instruments and enable the incorporation of automated functions at the early stage of technique development. Here, we exemplify this advantage of open-source electronics while prototyping an automated analytical device. Fizzy extraction takes advantage of the effervescence phenomenon to extract semi-volatile solutes from the liquid to the gas phase. The entire fizzy extraction process has been automated by using three Arduino-related microcontrollers. The functions of the developed autonomous fizzy extraction device include triggering the analysis by a smartphone app, control of carrier gas pressure in the headspace of the sample chamber, displaying experimental conditions on an LCD screen, acquiring mass spectrometry data in real time, filtering electronic noise, integrating peaks, calculating the analyte concentration in the extracted sample, printing the analysis report, storing the acquired data in non-volatile memory, monitoring the condition of the motor by counting the number of extraction cycles, and cleaning the elements exposed to the sample (to minimize carryover). The performance of this automated system has been evaluated using standards and real samples.

1. Introduction

The execution of most instrumental analysis methods requires a considerable amount of human effort. Typically, raw samples are first extracted to eliminate complex matrices that could interfere with the detection process or even contaminate the detector. Many of the available extraction protocols are performed manually by skilled technicians. Some of the more common procedures are automated with the aid of commercial robots, particularly autosamplers (robots with a small number of axes of freedom) that facilitate liquid handling [1, 2]. Such automated sample processing workflows decrease the amount of human labor. However, the operational flexibility of commercial platforms is restricted, what limits the incentive of analysts to develop completely new sample preparation approaches. Manual operation incurs lower overall performance of the newly developed methods and decreases their competitiveness with the established analytical methodology.

The recent notion of the "Industrial Revolution 4.0" inspires chemists

to create prototypes of new analytical instruments that are customized to meet specific requirements [3, 4]. Open-source electronic modules facilitate prototyping complex analytical instruments by non-engineers and enable incorporating automated functions from the very beginning of the inventive process (see, for example, refs. [2, 4, 5, 6, 7, 8]). The inventors can choose from a range of microcontroller boards with diverse specifications. The most popular family of open-source electronic modules is called Arduino [9]. The variety of functionalities provided by these modules make it appealing to construct fully automated and integrated analytical systems, which can be customized to match specific requirements at low cost. Due to the popularity of Arduino modules, one can readily find suitable code examples for these modules.

Gas bubbles have been utilized in analytical chemistry in different ways. For instance, in sparging-based extraction methods, gas is constantly passed through a liquid sample to promote the transfer of solutes to the gas phase [10, 11]. This approach provides a prolonged supply of gas-phase sample for analysis. To increase the detector
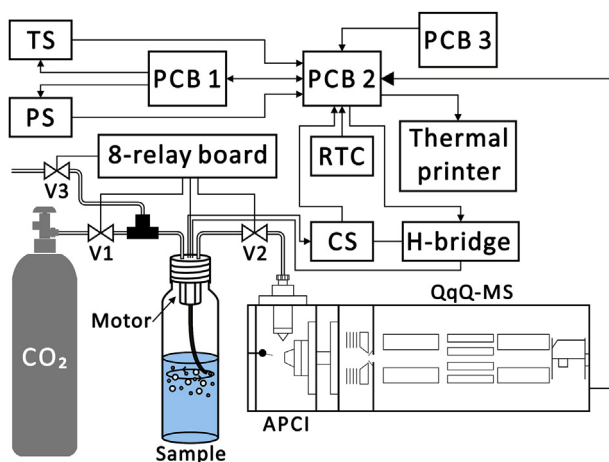
Fig. 1. Simplified scheme for the fizzy extraction system, including a block diagram of the electric control unit. Acronyms: TS – temperature sensor; PS – pressure sensor; RTC – real time clock (*N.B.* date and time are used to generate file names); CS – motor current sensor.

response, one needs to trap the gaseous analytes first and then release them as a pulse [12, 13, 14]. Alternatively, one can saturate the liquid sample with a gas and then decompress the sample to induce effervescence. The large number of bubbles produced in this process extract the volatile species from the liquid to the gas phase. The resulting pressure difference then assists the delivery of the extracted gas-phase analytes to an on-line detector in a short period of time. This technique—called "fizzy extraction"—simplifies and shortens sample preparation [15, 16]. However, it requires precise control of the gas pressure and timing, during which this pressure is applied to the sample (among other necessary functions). This kind of control could hardly be achieved manually. Thus, in the very beginning of the technique's development, it was clear that some kind of electronic control was necessary.

In this report, we demonstrate the possibility of building a prototype of an autonomous system comprising sample preparation and detection, which is equipped with multiple automated functions thanks to the implementation of such open-source microcontrollers. The functions of the developed fizzy extraction device include: triggering the analysis by a smartphone app, control of carrier gas pressure in the headspace of the sample chamber, displaying the experimental conditions on an LCD screen, acquiring mass spectrometry data in real time, filtering electronic
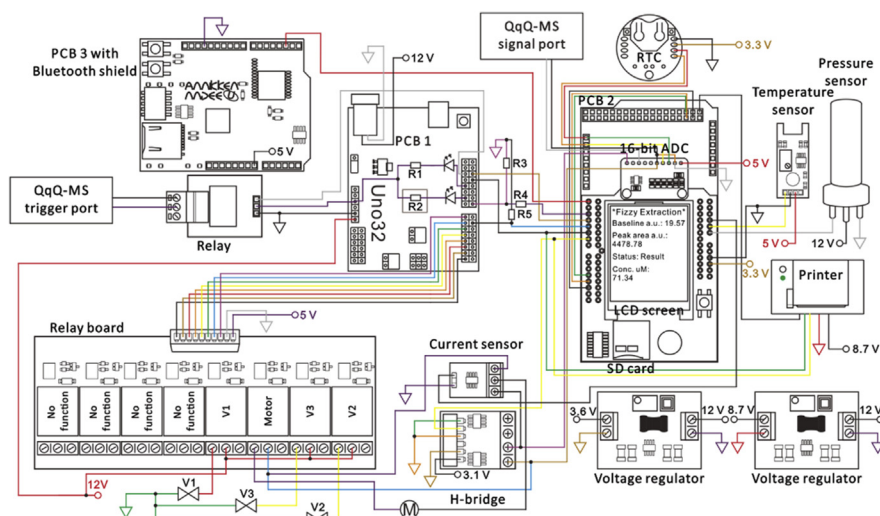

Fig. 2. Electronic schematic of the control unit used to operate the fizzy extraction system. The resistances of R1 and R2 are 470 Ω; R3 and R5, 4.7 kΩ; and R4, 1.5 kΩ.
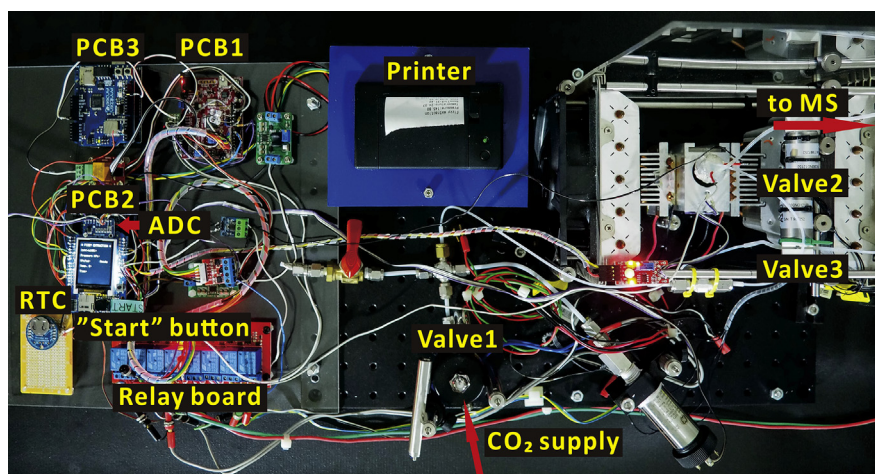

Fig. 3. Photograph of the assembled automated fizzy extraction system including the electronic control unit.

noise, integrating peaks, calculating the analyte concentration in the extracted sample, printing the analysis report, storing the acquired data in the non-volatile memory, monitoring the condition of the motor by counting the number of extraction cycles, and cleaning the elements exposed to the sample (to minimize carryover).

2. Experimental

2.1. Materials

Limonene was from Sigma-Aldrich/Merck (St. Louis, MO, USA). Myrcene was from Acros Organics (Geel, Belgium). Terpinene was from Sigma-Aldrich/Merck (St. Louis, MO, USA). Citronellal was from Alfa Aesar (Ward Hill, MA, USA). 1,8-Cineole was from Alfa Aesar (Ward Hill, MA, USA). Water (LC-MS grade) was from Merck (Darmstadt, Germany). Ethanol ($\geq$99.8% GC grade) was from Honeywell (Muskegon, MI, USA). The chemical standards were prepared in 5% ethanol/water. The concentrations of limonene standard were: 6.0×10^{-6} M, 1.5×10^{-5} M, 3.0×10^{-5} M, 6.0×10^{-5} M, 1.5×10^{-4} M, 3.0×10^{-4} M, and 4.5×10^{-4} M. The concentrations of 1,8-cineole standard were: 5.5×10^{-6} M, 1.4×10^{-5} M, 2.8×10^{-5} M, 5.5×10^{-5} M, 8.3×10^{-5} M, 1.1×10^{-4} M, and 1.7×10^{-4} M. The concentrations of myrcene standard were: 3.0×10^{-7} M, 4.5×10^{-7} M, 6.0×10^{-7} M, 9.0×10^{-7} M, 1.5×10^{-6} M, 3.0×10^{-6} M, and 6.0×10^{-6} M. The concentrations of citronellal standard were: 1.4×10^{-6} M, 2.8×10^{-6} M, 5.5×10^{-6} M, 1.4×10^{-5} M, 2.8×10^{-5} M, 4.1×10^{-5} M, and 5.5×10^{-5} M. The real samples included in this study were orange juice and saliva. For orange juice, half of an orange was squeezed on a kitchen squeezer. The orange juice sample was diluted 100 $\times$ with 5% ethanol/water. Saliva specimens were obtained by spitting from a volunteer who had recently used mouthwash. They were diluted 10$\times$ with 5% ethanol/water.

2.2. Apparatus and procedure

The starting point for the development of this automated system was the previous version of the fizzy extraction prototype [15, 16]. In the present work, a number of automated functions have been incorporated. The delivery of carrier gas to the sample headspace is controlled by a Chipkit Uno32 (Digilent, Pullman, WA, USA; PCB 1). PCB 1 triggers the relay board, which supplies electric currents to various actuators (a solenoid valve – V1, two pinch valves – V2 and V3, and a miniature DC motor; Figs. 1, 2, and 3). The newly added microcontrollers are an Arduino Mega (PCB 2) and an Arduino Uno (PCB 3). PCB 2 is fitted with a miniature LCD screen shield incorporating a microSD card slot and a joystick (1.8 inch; Adafruit, New York, NY, USA) as well as mini thermal receipt printer (Adafruit). It is also fitted with an external analog/digital converter (ADC, ADS1115, 16 bit, 4 channels; Adafruit) and an ultra-precise real time clock (ChronoDot v2.1, Adafruit). PCB 3 is fitted with a stackable shield – Andee U (Annikken, Singapore). The purpose of this shield is to communicate with a mobile device via Bluetooth and enable the ability to trigger the analysis remotely using a smartphone. The cost of building this prototype was ~1400 USD (cf. Table 1). Because the system was mostly developed by a chemistry graduate student within two years, the development did not incur high labor cost (total stipend of the student: ~ 6000 USD). We have not applied for a patent for this invention, and are not selling the license for the microcontroller programs for profit.

The automated fizzy extraction system was coupled with a triple quadrupole (QQQ) mass spectrometer (LCMS-8030; Shimadzu, Tokyo, Japan) operated in the atmospheric pressure chemical ionization (APCI; Duis source) and single reaction monitoring (SRM) modes. The mass spectrometer was controlled by the LabSolutions software (version 5.82, Shimadzu).

2.3. Microcontroller programs

The operation of the fizzy extraction system is controlled by programs written in C++ and deployed on the three PCBs (cf. Fig. 4). Briefly, the fizzy extraction process is started by pushing the joystick on the LCD shield (PCB 2) or pressing a virtual button on the smartphone app, which communicates via Bluetooth with the shield on PCB 3. That signal triggers the extraction routine programmed in PCB 2. At that point, PCB 2 toggles PCB 1, which controls all the actuators involved in the extraction process (the valves, motor, and the start of the data acquisition by the mass spectrometer). The fizzy extraction routine consists of the following steps:

(1) recording and zeroing baseline, 6 s, V2 open, V1 and V3 closed;
(2) headspace flushing, 60 s, V1 and V2 open, V3 closed;

Table 1
Bill of materials used to construct the automated fizzy extraction device (note: 1 USD = 30.655 NTD, as of 9 July, 2018).

| Item	Supplier	Unit	Number of units	Unit price/ NTD	Total cost/ NTD
Arduino Uno	Centenary Materials	PC	1	275	275
Arduino Mega	Centenary Materials	PC	1	490	490
Annikken Andee	Annikken	PC	1	79	79
ChipKit Uno32	Digipart	PC	1	681	681
Adafruit 1.8″ Color TFT Shield w/ microSD and Joystick	Adafruit	PC	1	1068	1068
Real time clock	Adafruit	PC	1	535	535
16-bit ADC	Adafruit	PC	1	457	457
Printer	Adafruit	PC	1	1527	1527
Pressure sensor	GE electric	PC	1	11000	11000
Temperature sensor	Centenary Materials	PC	1	75	75
Relay board	Centenary Materials	PC	1	260	260
Relay	Centenary Materials	PC	1	55	55
Voltage regulator	Kinsten Materials	PC	2	100	200
Current sensor	eBay	PC	1	36	36
H-bridge	Kinsten Materials	PC	1	50	50
Valve (V1)	Thai Xin Machinery	PC	1	606	606
Valve (V2, V3)	ASCO	PC	2	4830	9660
Metal rod	Thorlabs	PC	5	190	950
Metal rod	Thorlabs	PC	2	175	350
Metal rod	Thorlabs	PC	1	153	153
Metal support	Thorlabs	PC	2	305	610
Metal support	Thorlabs	PC	1	256	256
Acrylic board	Acrylic Studio, Hsinchu	PC	2	100	200
T-junction	Swagelok	PC	1	924	924
Union Cross	Swagelok	PC	1	2270	2270
Breadboard	Newport	PC	1	8000	8000
Glass vial	Thermo	PC	1	20	20
Holder	NTHU workshop	PC	1	800	800
Tubing	Super Chroma	M	1	683	683
Motor	Centenary Materials	PC	1	60	60
Cable	Centenary Materials	M	3	120	360
Others (nuts, screws)	Centenary Materials	PK	1	500	500
Total					**43190**
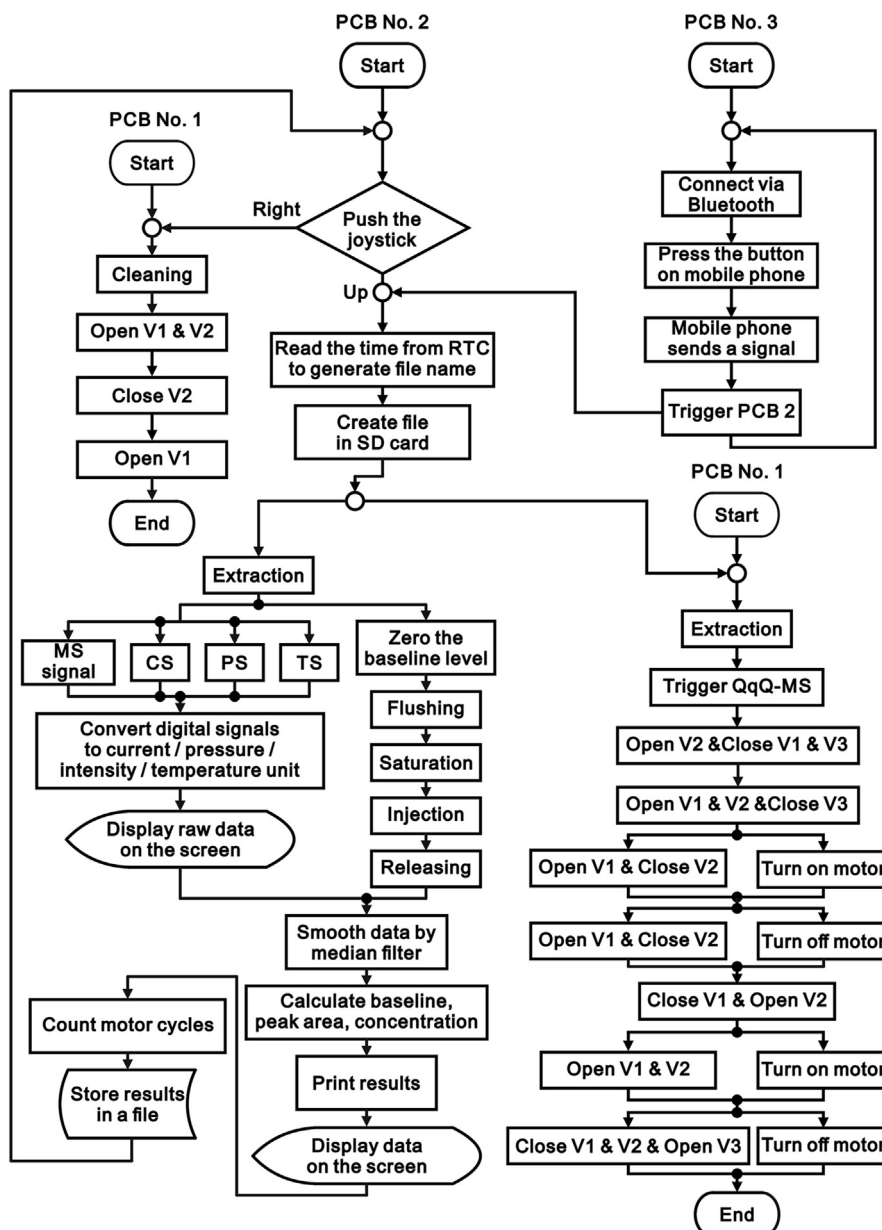
Fig. 4. Workflow for the fizzy extraction procedure.

(3) saturation of sample with carbon dioxide, 60 s, V1 open, V2 and V3 closed, motor on;
(4) equilibration, 1 s, all valves closed;
(5) extraction and injection, 2 s, V2 open, V1 and V3 closed;
(6) extraction and injection, 28 s, V1 and V2 open, V3 closed, motor on;
(7) releasing the pressurized gas from the headspace, 24 s, V3 open, V1 and V2 closed.

When the extraction procedure is initiated, PCB 2 creates a new file on the microSD card. The file name is generated based on the actual time provided by the real-time clock module. Subsequently, PCB 2 records the signal supplied by the analogue output of the mass spectrometer and other experimental parameters such as temperature and pressure. The duration of one loop is 0.25 s. In this time, five data points are recorded, and a median value is calculated. The first data point from the mass spectrometer is used to zero the baseline. Every raw value is

then converted to a value expressed in arbitrary units (a.u.), which are approximately equivalent to the arbitrary units used by the original software of the mass spectrometer, and saved in a data array. At the same time, the carrier gas pressure and ambient temperature are also measured and stored. After the fizzy extraction routine is over (end of the loop), the data array with the temporal MS data is further processed. The median filter is applied again (window size: 5 data points). An average value is computed for the detector baseline (30 s during the saturation step). The baseline value is subtracted from every data point within the MS temporal peak (unless the data point is lower than the baseline value), and the results of the subtraction are summed and multiplied by 0.25 s to give the peak area. The parameters of the linear calibration equation are loaded from the calibration file saved on the microSD card, and the concentration is computed based on the peak area value. The raw data and processed results are stored in a result file on the microSD card. The final result is also displayed on the LCD screen for 10 seconds and printed immediately. At that point, the system is
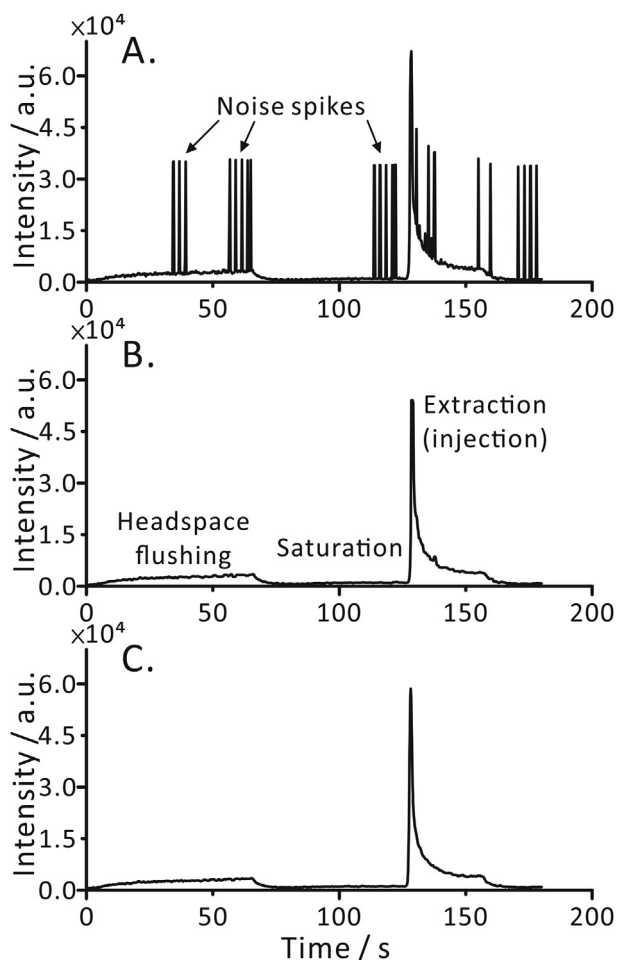
Fig. 5. The effect of a median filter on signal quality. (A) Unfiltered signal recorded by Arduino. (B) The same signal after applying median filter. (C) The corresponding dataset recorded by the original software of the mass spectrometer. Sample: 5.5×10^{-5} M 1,8-cineole in 5% ethanol/water solution. The SRM data were recorded at m/z 155→81.

conversion factor was 1 unit μV^{-1} (for limonene: 0.1 a.u. μV^{-1}).

3. Results and discussion

3.1. Development of the automated fizzy extraction system

The development of this automated fizzy extraction system entailed a series of preliminary tests. Most of the technical issues—related to the compatibility of the electronic modules—were addressed by referring to online tutorials on open-source electronics and programming. One of the issues to address was the limited resolution of the ADC built into the Arduino Mega microcontroller board (PCB 2), which was 10 bit. Such a low resolution did not warrant faithful representation of the MS temporal peak shape. Therefore, we decided to implement an external 16-bit ADC board equipped with a gain amplifier. The amplification factor was set to 4. These settings enabled the acquisition of the analogue SRM signal outputted from the mass spectrometer at satisfactory resolution. Much attention was also dedicated to processing the raw analogue signal obtained from the mass spectrometer. We found that the signal was dominated by electronic noise. This kind of noise is quite common in analogue signal transmission and partly originates from the laboratory environment [17]. Thus, signal filtering was necessary to attain temporal datasets comparable to those displayed by the mass spectrometer's software. To remove the random signal noise (including spikes), we implemented two software-based median filters (Fig. 5).

It should be noted that the fizzy extraction process requires stirring the sample at two stages – first during saturation of the sample with the carrier gas and later during effervescence. We realized that the speed of rotation of the stirring spindle depends on the condition of the motor. As the motor ages, its performance decreases, which affects the outcome of the extraction. A current sensor was introduced to the motor circuit, and the number of extraction cycles was also recorded on the microSD card to follow the condition of the motor. Moreover, the motor voltage can be adjusted from the software level to tune the rotation speed. Following these improvements, the operation of the automated fizzy extraction proceeded seamlessly (**Movie S1** in 'Appendix A. Supplementary data'). The LCD screen displayed the parameters of the fizzy extraction in real time (Fig. 6A). In this prototype, the extraction could be started by pushing the joystick, or remotely from an Android app (Fig. 6D). It is
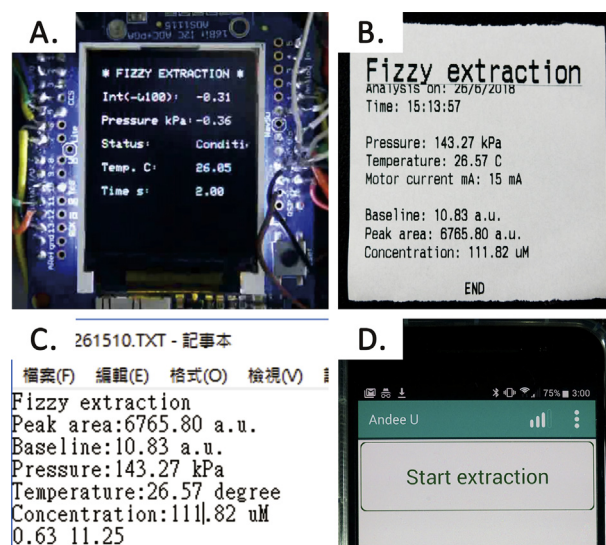
ready to analyze a new sample.

By pushing the joystick to the right hand side, a special washing program is deployed to remove residues of the old sample from the stirring spindle and minimize carryover. Furthermore, in order to achieve repeatable results, the condition of the stirring motor is monitored. First, in the course of the experiment, PCB 2 measures the motor current (with the aid of a current sensor) and then shows the result on the final analysis report. A major malfunction of the motor would cause a dramatic decrease or increase of this value. The normal current value is in the range of 10–50 mA. Second, based on our experience, after 500 extraction cycles, the stirring motor's rotation is unstable, and a characteristic acoustic noise is audible. To track the level of motor usage, the PCB 2's program stores the information on the number of extraction cycles in the microSD card for the user's reference.

2.4. Mass spectrometry parameters

The potential of the APCI needle was 4.5 kV. The flow rate of the nebulizer gas was 2.5 L min^{-1}. The flow rate of the drying gas was 5 L min^{-1}. The temperature of the desolvation line was 250 °C. The collision gas was argon. Its pressure was set to 230 kPa. The collision voltages were −20 or −15 V (for different compounds). The raw analogue signal was output from the mass spectrometer and supplied to an analogue input of the ADC connected to PCB 2. The signal-to-voltage

Fig. 6. Different ways of interacting with the user: (A) LCD screen; (B) report printed by the thermal printer; (C) screen of the text editor displaying ASCII file saved by the extraction system on the microSD card; (D) smartphone screen with the interface for triggering the fizzy extraction.
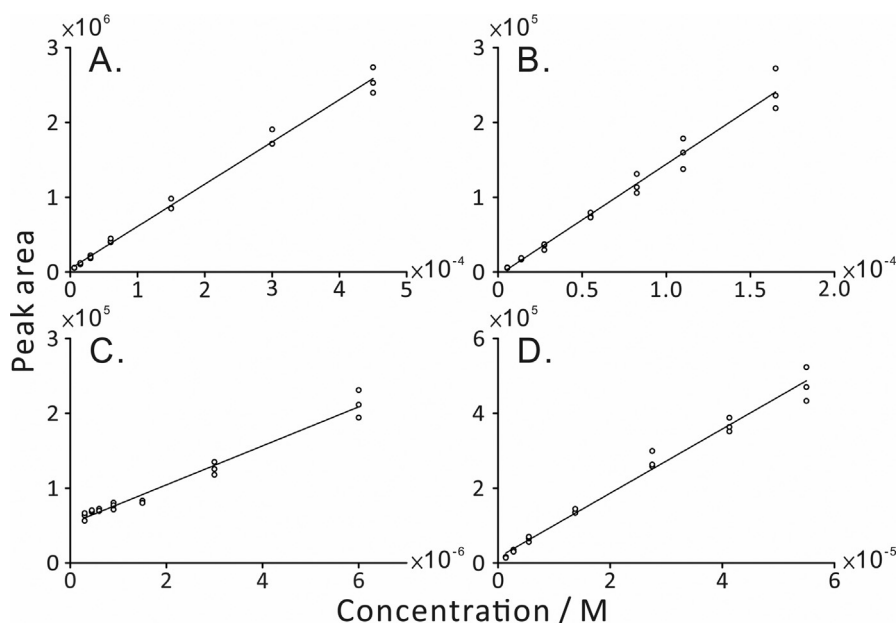
Fig. 7. Calibration plots for four compounds. (A) limonene; (B) 1,8-cineole; (C) myrcene; (D) citronellal. For calibration curve equations, see Table 2.

Table 2
Analytical performance results. For calibration plots, see Fig. 7. LOD – limit of detection. LOQ – limit of quantification ($3 \times$ LOD).

Compound	m/z	LOD/M	LOD/mg L^{-1}	LOQ/M	LOQ/mg L^{-1}	Calibration equation (units of C: M)	R^2
limonene	137→81	2.89×10^{-5}	3.94	8.57×10^{-5}	11.67	$PA = (5.65 \times 10^9 \pm 1.06 \times 10^8)C + (4.48 \times 10^4 \pm 2.26 \times 10^4)$	0.993
1,8-cineole	155→81	1.80×10^{-5}	2.78	5.41×10^{-5}	8.34	$PA = (1.49 \times 10^9 \pm 4.93 \times 10^7)C - (4.58 \times 10^3 \pm 4.18 \times 10^3)$	0.978
myrcene	137→81	7.20×10^{-7}	0.10	2.16×10^{-6}	0.29	$PA = (2.60 \times 10^{10} \pm 9.98 \times 10^8)C + (5.22 \times 10^4 \pm 2.63 \times 10^3)$	0.971
citronellal	155→81	5.39×10^{-6}	0.83	1.62×10^{-5}	2.50	$PA = (8.59 \times 10^9 \pm 2.39 \times 10^8)C + (1.47 \times 10^4 \pm 6.83 \times 10^3)$	0.985

imaginable that—following further modification—the extraction process can start spontaneously, circumventing the need to trigger it by the user. After the extraction, the final results were displayed on the LCD screen (Fig. 6A) and printed by a miniature thermal printer (Fig. 6B). The digital data record could be retrieved from the microSD card after analysis (Fig. 6C).

3.2. Characterization of the automated fizzy extraction system

The developed automated system was first tested using standard samples. Calibration plots were constructed for four test analytes: limonene, 1,8-cineole, myrcene, and citronellal (Fig. 7, Table 2). The analytes were prepared in 5% ethanol/water solution. The total sample volume was 10 mL. The data points generally demonstrated linear characteristics. It is pleasing to note that the peak areas computed by the developed system and the peak areas obtained by integrating the ion current peaks recorded by the original software of the mass spectrometer are well-correlated (Fig. 8). The limits of detection (LODs) for the test analytes using the developed system range from 7.20×10^{-7} to 2.89×10^{-5} M (calculated based on the slopes, intercept standard deviations of the calibration lines, and residual standard deviation [18]; Table 2). The intraday repeatabilities ranged from 4.7 to 10.4% (relative standard deviation (RSD), $n = 10$; Table 3). The repeatabilities of the results obtained by the Arduino program were comparable with the corresponding results obtained by the original instrument software (similar RSDs), what shows that the peak integration algorithm—implemented in the Arduino program—provides satisfactory performance. The repeatabilities could potentially be improved further by implementing isotopically labeled internal standards.

3.3. Application of the automated fizzy extraction in the analysis of real samples

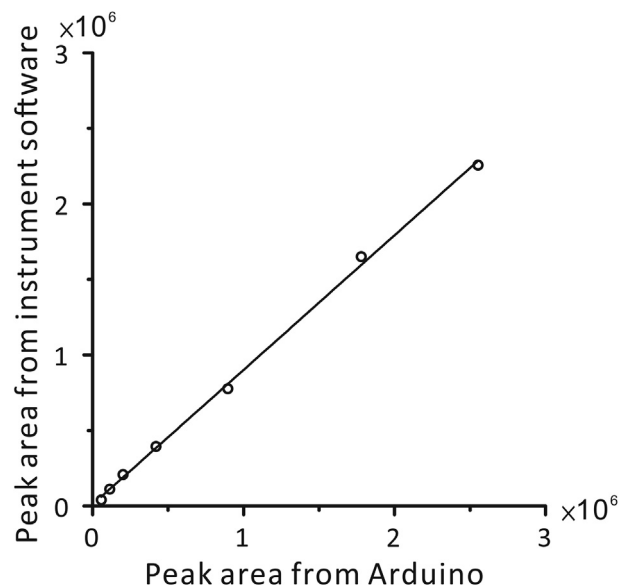The automated fizzy extraction is capable of calculating analyte

Fig. 8. The correlation of peak area computed by the Arduino script and the instrument software. The solid line is the result of linear regression, and it is described by the equation $A_I = (0.89 \pm 0.01)A_A + (1.03 \times 10^4 \pm 1.79 \times 10^4)$.

Table 3

Repeatabilities of analyses conducted by the fizzy extraction system with data analysis conducted by the Arduino script and with data analysis conducted by the commercial software.

Compound	Conc./M	Repeatability with Arduino (RSD/%) $n = 10$	3-day variability with Arduino (RSD/%)	Repeatability with commercial software (RSD/%) $n = 10$	3-day variability with commercial software (RSD/%)
limonene	6.00×10^{-5}	7.0	12.3	10.2	17.9
1,8-cineole	5.50×10^{-5}	10.4	23.5	7.7	27.2
myrcene	6.00×10^{-6}	4.7	9.2	9.6	28.2
citronellal	1.38×10^{-5}	8.2	14.7	7.5	24.9

concentrations immediately after extraction and detection. To exemplify potential applications in food chemistry, the platform was further applied to analyze limonene in orange juice diluted $100\times$ in 5% ethanol/water solution to minimize the possible matrix effects (Fig. 9A). The system automatically computed the concentration of limonene using the calibration data stored on the microSD card. After multiplying that concentration by the dilution factor, the final concentration of limonene in orange juice was measured as $3.89 \times 10^{-3} \pm 0.30 \times 10^{-3}$ M ($n = 3$). The concentration of limonene in orange juice has previously been reported by gas chromatography (GC) to be both 1.58×10^{-3} M and 9.32×10^{-3} M [19, 20]. These reference values are satisfactorily close to the value measured by the automated fizzy extraction system. However, the concentration of limonene in orange juice is expected to vary depending on the cultivar, climate, season, and other factors. While the current work encompasses automation of fizzy extraction, to validate the analytical method, one would further need to perform reference measurements.

To further demonstrate suitability of automated fizzy extraction to analyze selected biological matrices, 1,8-cineole was detected in saliva obtained from volunteer who had previously used mouthwash. Before the sample collection, the volunteer flushed their mouth with water. After 30 minutes, they rinsed their mouth with ~20 mL mouthwash for 30 seconds, following the use guidelines adhered onto the bottle. Saliva specimens were then collected 1, 5 and 10 minutes after rinsing. The collected saliva specimens were diluted $10\times$ in 5% ethanol/water solution to minimize the possible matrix effects and to ensure that sample volumes match the required system volume (10 mL). The unprocessed fizzy extraction data show that the 1,8-cineole peak decreases over time; after 5 minutes, the peak disappears (Fig. 9B, C and D), indicating evaporation, absorption, and ingestion of the mouthwash components present in saliva fluid. The concentration of 1,8-cineole in the saliva specimen (obtained 1 minute after rinsing mouth) was computed based on the calibration data to be 3.55×10^{-4} M. In principle, a similar experiment can be performed by GC and using other sampling and extraction techniques. Automated fizzy extraction, performed in conjunction with APCI-MS, simplifies the analysis procedure to some extent.

Furthermore, the recoveries of limonene from dilute orange juice (spiked concentration: 6×10^{-5} M) and 1,8-cineole from dilute mouthwash (spiked concentration: 5.5×10^{-5} M) were computed as $112 \pm 6\%$ and $88 \pm 3\%$, respectively. The deviation of recoveries from 100% is probably due to the matrix effect that occurs when analyzing complex samples (juice, saliva), which may contain various other compounds: volatile and non-volatile, ionizable and non-ionizable. Notably, this matrix effect is not related to the automation described in this report but to the extraction process and on-line detection. The matrix effect can potentially be reduced by utilizing isotopically labeled internal standards and incorporating a separation step immediately before MS detection. While the present study focuses on automation of the fizzy extraction system, work is currently underway to hyphenate fizzy extraction with other detection systems than the APCI-QQQ-MS
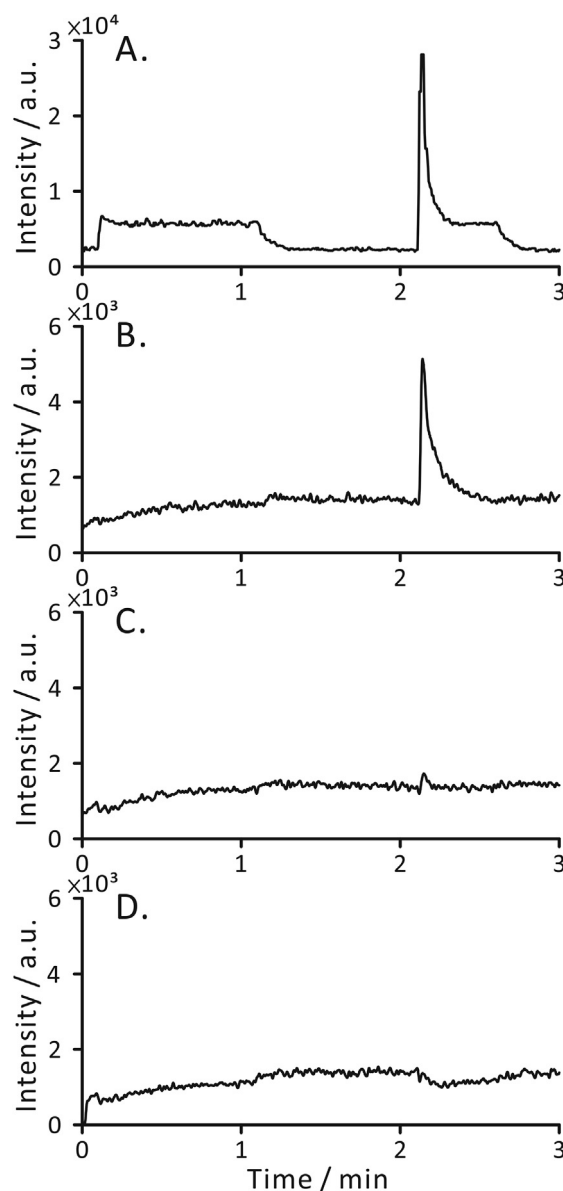

Fig. 9. Typical results obtained with the automated fizzy extraction system: (A) Limonene in $100\times$ diluted orange juice in 5% ethanol/water solution (m/z $137 \rightarrow 81$); (B-D) 1,8-cineole in $10\times$ diluted saliva (in 5% EtOH water solution) obtained from a volunteer who had previously rinsed their mouth with mouthwash (m/z $155 \rightarrow 81$). The saliva specimens were obtained (B) 1 min, (C) 5 min, and (D) 10 min after rinsing.

implemented here.

It should be noted that analyses of volatile solutes present in food and clinical matrices are often performed by techniques such as static and dynamic headspace analysis, purge-closed-loop, purge-and-trap, single droplet microextraction, and solid-phase microextraction. These sampling/extraction techniques are often combined with GC. Notably, food and clinical analysis are highly regulated areas. Therefore, for fizzy extraction to find applications in these areas, further validation studies are required.

4. Conclusions

While volatile organic compounds are typically analyzed by GC preceded by various sampling and (micro)extraction steps, fizzy extraction in conjunction with direct MS provides an alternative to these conventional procedures. Automation is a way to increase practicality of fizzy extraction in analytical applications. Open-source hardware and software can readily be used by chemists to bring newly developed methods to the next level and to operate them seamlessly – in a similar manner to the way one operates well-established and commercial analytical instruments. We have demonstrated the possibility of automating the fizzy extraction procedure by implementing open-source electronic modules and programming in C++. Assembling this automated prototype was straightforward for the analysts without formal training in engineering. The automation of this relatively new sample preparation scheme eliminates the influence of the human factor on the reproducibility of the analysis. Because of its low cost and simple design, the automated fizzy extraction device can be replicated by other chemists and used to perform analyses of volatile species inside and outside the chemical laboratory; for example, in conjunction with one of the available miniature mass spectrometers (*e.g.* quadrupole, ion trap, or and time-of-flight fitted with APCI source), to make the entire system portable, and enable field analyses. Such a portable system will need to be equipped with an additional control module controlling intrinsic features of the mass analyzer.

Declarations

Author contribution statement

Hao-Chun Yang: Performed the experiments; Analyzed and interpreted the data; Wrote the paper.

Chun Ming Chang: Analyzed and interpreted the data.

Pawel Urban: Conceived and designed the experiments; Contributed reagents, materials, analysis tools or data; Wrote the paper.

Funding statement

Competing interest statement

The authors declare no conflict of interest.

Additional information

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