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Short communication

# A flow-batch analyzer using a low cost aquarium pump for classification of citrus juice with respect to brand

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ABSTRACT

This paper proposes a novel flow-batch analyzer (FBA), which employs a compact, low-cost aquarium air pump as an alternative to a peristaltic pump. The feasibility of using this simple propulsion device is demonstrated in a case study involving the classification of citrus juice samples with respect to brand. For this purpose, UV–vis spectra and SIMCA (soft independent modelling of class analogies), PLS-DA (Partial Least Squares for Discriminant Analysis) and SPA-LDA (Linear Discriminant Analysis with variables selected by the Successive Projections Algorithm) are employed. Good classification results were obtained, thus indicating that the proposed FBA system is a viable alternative to the use of more costly peristaltic pumps. In addition, the smaller size and weight of the aquarium pump are useful features for the construction of portable FBAs to be deployed in field applications.



## 1. Introduction

Automatic methods are widely used in several areas, such as clinical, environmental, pharmaceutical and food analysis. Such methods can be implemented in an efficient manner through the use of flow injection analysis systems, which facilitate sample pre-treatment, management of reagents, monitoring of the analytical signal, reduction of human effort, more precise analysis and increase in the sample rate [1,2]. Nevertheless, this type of system has some disadvantages, such as the need for frequent recalibration and manual adjustments, low sensitivity due to sample dispersion and inefficient homogenization, as well as the generation of a large volume of residues due to the use of carrier fluid [3]. These inconveniences motivated the development of flow-batch analyzers (FBA) [4].

FBA is an automated system that uses an instantaneous stop chamber and integrates batch and flow methods by means of programmed multi–commutation [5]. The main component is the mixing chamber where the whole analytical process, including fluids addition, sample pretreatment, homogenization, precipitation, extraction, preparation of standard solutions, and detection, takes place under total control of the software [6]. The sample is processed seamlessly with less manipulation, consumption of reagents and samples, waste generation and chance for human error [3].

Most FBA systems described so far employ peristaltic pumps for fluid propulsion [3,7–9]. Such pumps have multiple channels and can be used for either propulsion or aspiration, without direct contact of the fluid with mechanical components. However, these propulsion devices are relatively costly ( > US$ 4000). Moreover, their size and weight hinder the deployment of portable FBA systems for field use. To circumvent these inconveniences, other propulsion alternatives for FBA have been exploited, such as piston propulsion [10,11] and solenoid micro-pumps [12,13].

Within this context, the present work proposes a new flow-batch analyzer, which employs a compact, low-cost propulsion system driven by an aquarium air pump (~US$ 15). The proposed analyzer is applied to the screening analysis of citrus juice samples with respect to brand by using UV–vis spectrometry and chemometrics techniques. More specifically, SIMCA (Soft Independent Modelling of Class Analogies) [14], PLS-DA (Partial Least Squares for Discriminant Analysis) [15] and SPA-LDA (Linear Discriminant Analysis with variables selected by the Successive Projections Algorithm) [16,17] are employed to discriminate the UV–vis spectra of the juice samples.

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## 2. Experimental

### 2.1. Samples

This work involved 150 samples of six commercial brands of processed citrus juice (denoted by I1–I6) and 20 samples of fresh citrus juice (denoted by *N*), which were acquired in the city of João Pessoa (PB, Brazil). The samples for each brand were taken from different lots.

Due to the strong absorption of the citrus juices in the UV–vis range, all samples were diluted by addition of water in the proportion 1:70 (v/v). Water was distilled and deionized by using a Milli-Q Plus system (Millipore).

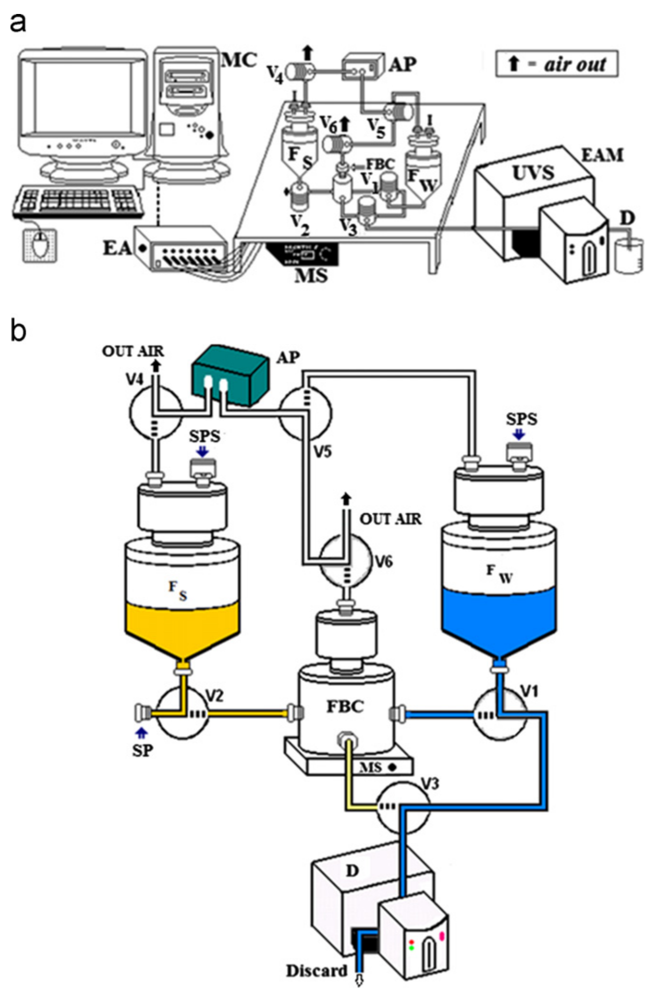


**Fig. 1.** (a) Proposed flow-batch analyzer: *EA*=electronic actuator, *FBC*=flow-batch chamber, *MS*=magnetic stirrer, *AP*=aquarium pump, *V*1–*V*6=solenoid valves, $F_S$ and $F_W$=sample and water flasks, *SP*=screw plug, *SPS*=screw plug with septum, *MC*=microcomputer, *D*=UV–vis spectrophotometer. (b) Simplified diagram of the flow-batch analyzer with indication of the two possible valve configurations (ON and OFF).

### 2.2. Apparatus

The proposed FBA system is depicted in Fig. 1a. The system comprises six *three-way* solenoid valves (Cole-Parmer), an aquarium pump (Boyu S-2000A Duplo), hermetically sealed flasks for the sample and diluent, a PTFE (Teflon) flow-batch chamber (FBC) with a magnetic bar in its interior, a magnetic stirrer (Hanna Instruments, model HI 190M) and a quartz flow cell (Hellma) with optical path of 1.0 cm. The UV–vis spectra are acquired by using a Hewlett Packard 8453 spectrophotometer with photodiode array in the range 190–1100 nm with a resolution of 1 nm.

A microcomputer is employed for data acquisition and control of the flow-batch analyzer with software developed in the LabView 5.1 platform. An electronic actuator is used to switch the solenoid valves and to activate/deactivate the aquarium pump. Fig. 1b presents a simplified diagram of the analyzer. In this diagram, all valves are shown in the OFF position. When a valve is switched to the ON position, its output is moved to the dotted line.

### 2.3. Procedure

Initially, the sample flask $F_S$ is washed with the sample under analysis. For this purpose, 10 ml of the sample are introduced through the septon of the screw plug at the top of the flask by using a syringe. The sample is then drained by removing the screw plug at the bottom. This procedure is always repeated three times for each new sample to be analyzed. After this cleaning step, another 10 ml of the sample are introduced for analysis. The water flask $F_W$ is also filled for use in the subsequent cleaning, dilution and measurement steps, as summarized in Table 1. Since the volumes added to the flow-batch chamber FBC are proportional to the valve opening times, the analytical procedure is described in terms of time rather than volume.

In Step 1, valves *V*1, *V*2, *V*4 and *V*5 are simultaneously switched ON for 5.0 s in order to fill the channels between valves *V*1, *V*2 and the FBC. Step 2 consists of the cleaning and draining of the FBC. For this purpose, valves *V*1 and *V*5 are switched on during 5.0 s to introduce water into the FBC and then valves *V*3 and *V*6 are switched on for 10.0 s to discard the FBC content. This cleaning and draining procedure is carried out in triplicate. Steps 1 and 2 are repeated in the analysis of every new sample.

In Step 3, valve *V*5 is switched on for 10.0 s in order to fill the UV–vis spectrophotometric flow cell with water for the blank signal measurement.

In Step 4, valves *V*1, *V*4 and *V*5 are switched on for 6.90 s and valve *V*2 is simultaneously switched on for 0.1 s in order to dilute the sample in the proportion 1:70 v/v. In Step 5, valves *V*3 and V6 are switched on for 10.0 s in order to fill the flow cell for the sample signal measurement.

Prior to the analysis of a new sample, the screw plugs at the top and bottom of the sample flask $F_S$ are removed and the flask is washed three times with water. The channel between $F_S$ and FBC is also drained and cleaned by reinserting the screw plugs, filling

**Table 1**
Sequence of steps in the operation of the flow-batch analyzer, with indication of the switch-on times (in seconds) of valves *V*1–*V*6.

| Step | Description | V1 | V2 | V3 | V4 | V5 | V6 |
|---|---|---|---|---|---|---|---|
| 1 | Channelfilling | 5.0 | 5.0 | – | 5.0 | 5.0 | – |
| 2 | Cleaning and draining of the flow-batch chamber | 5.0 | – | – | – | 5.0 | – |
| | | – | – | 10.0 | – | – | 10.0 |
| 3 | Blanksignalmeasurement | – | – | – | – | 10.0 | – |
| 4 | Sample dilution | 6.9 | 0.1 | – | 6.9 | 6.9 | – |
| 5 | Sample signal measurement | – | – | 10.0 | – | – | 10.0 |