



VAPOR IDENTIFICATION SYSTEM USING QUARTZ RESONATOR SENSOR ARRAY AND SUPPORT VECTOR MACHINE

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ABSTRACT

It has been developed a vapor identification system using gas sensor array and Support Vector Machine (SVM) pattern recognition. Sensor array consists of several quartz resonator sensors coated with different polymer materials in order to have a specific pattern to the vapor. In this study, the Field Programmable Gate Array was used as counters and other functions to interface the sensor array with a computer. Frequency change was measured by a counter with a period of one second. Vapors used in the experiment were kerosene, methanol, gasoline and alcohol. The data analysis was taken from the frequency changes after vapor injection. Sensors were cleaned to get the initial condition using nitrogen gas. For vapor data collecting, the measurements were performed eight times for each sample. The set of digital data was then stored as a database. Principle Component Analysis was used to visualize the performance of the sensor array to discriminate each vapor. The set of vapor pattern obtained by the sensor array was then identified by SVM algorithm. Experiment results showed that the SVM could identify each vapor with a success rate of 97.2%. The results of this study will be used for further research to detect the low concentrations of vapors contained in human breath for medical diagnoses.

Keywords: quartz resonator sensor array, SVM, vapor identification.

INTRODUCTION

To analyze or identify gas or vapor, many researchers usually use a tool that consists of a combination of a sensor array and pattern recognition. Quartz resonator is one of the vapor sensor based on the frequency shift of acoustic wave. Due to a small change of mass absorbed on the surfaces, so that in the chemical process; the type of sensor is used as vapor deposition probes [1]. The pattern of the normalized resonant frequency shifts is a typical for each vapor because each sensor is coated by polymer with a different partition coefficient. During the two months of measurements, the pattern changes of a normalized frequency shift have a mean level of reliability of 0.99 [2] [3]. A multichannel of

frequency counters interfaced to a computer through a serial communication has been implemented in a Spartan-3E Field Programmable Gate Array (FPGA). This design is used to detect changes in frequency caused by vapor that was supplied by the sensor module. The average interference error on each channel is 0.0029% [4].

To complete the vapor identification system, the device requires a data processing algorithm for extraction, classification and identification purposes. The Principle Component Analysis (PCA) method is often used for visualization of classification results in the identification system. This method is derived from factor analysis technique that aims to identify the structure of many variables into a simplified data. PCA is typically



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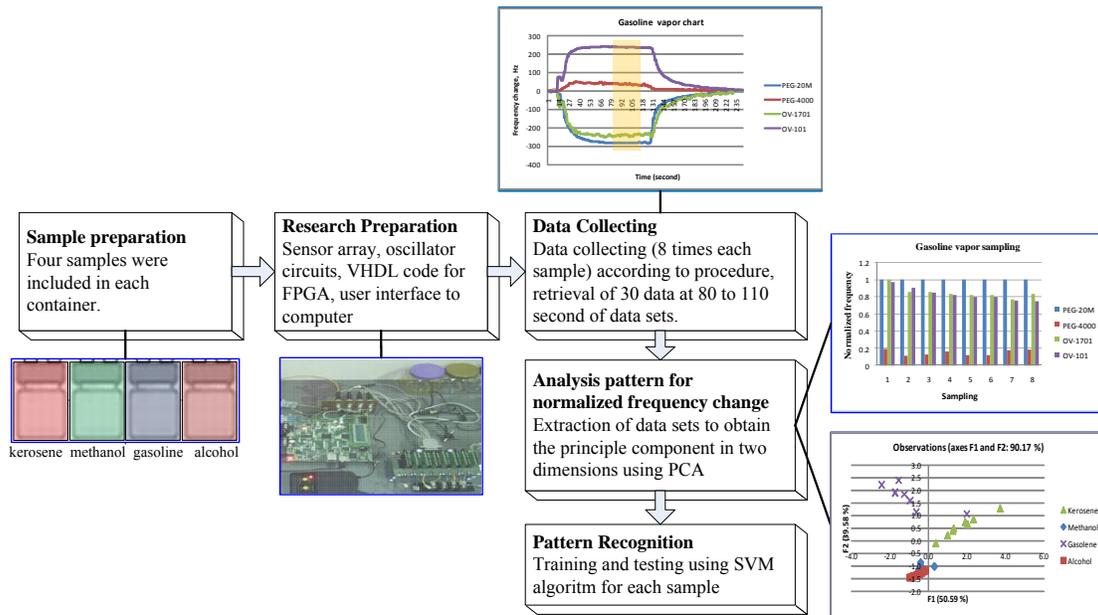


Figure-1. The research method.

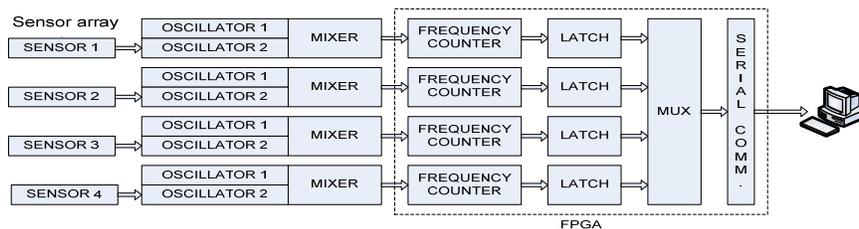


Figure-2. Block diagram of the system.

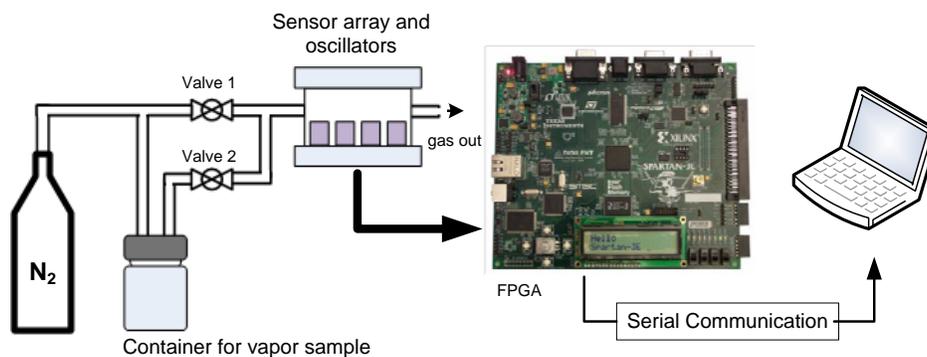


Figure-3. Block diagram of data collection equipment.

used not only to reduce the dimensionality of the data set but also maintains the characteristics of the data sets by maintaining several high-priority principal components and discard some low-priority principal component [5]. Other method recently receiving much attention as the state of the art in pattern recognition is Support Vector Machine (SVM) [6] [7], and it is considered better than Artificial Neural Networks (ANNs), especially in multi-class classification [8] [9] [10].

MATERIAL AND METHOD

Figure-1 describes the overall research methodology that has been done step by step. Each step describes activity that has been carried out and will be discussed more details in the following section. Block diagram of the system is shown in Figure-2 consisted of three parts: sensors, oscillators, mixers, FPGA blocks and a computer. The sensor is a quartz resonator having the fundamental resonance frequency of 20 MHz. This sensor



responds to gases adsorbed on the quartz resonator electrodes, by which the piezoelectric effect will change its oscillation frequency. Frequency change (ΔF) that occurs is proportional to the total mass of the adsorbed gas molecules expressed in the Sauerbrey equation: [11].

$$\Delta F = -2.3 \times 10^6 \cdot x F^2 \cdot \frac{\Delta M}{A} \quad (1)$$

where F is a base frequency (MHz), ΔM is the total mass of the adsorbed gas molecules (g/cm^2), A is an area of the electrode. Each quartz resonator sensor was coated with different polymers on the surface to form a certain pattern to the vapor. Polymer materials used in this experiment are OV1701, OV101, PEG20M and PEG4000. Each polymer material has a different polarity including non-polar, mid polar and polar, which is intended to be able to absorb a wide range of molecules contained in the vapor. The sensor oscillator is Pierce oscillator models [12] connected to the sensor to produce a square wave with a frequency of 20 MHz. The use of sensors with a fundamental frequency of 20 MHz causes interference among the channels so that the output frequency of the oscillator should be lowered. The mixer circuit produces an output that represents the difference between the two frequencies of sensor and reference oscillators. The reference oscillator behaves the source of constant frequency of 20 MHz. These mixer circuits uses D flip-flop 74HC74 followed by first order Passive RC Low-Pass Filter to block the higher frequency. Frequency counters are generally constructed from a series of flip-flop. Design of frequency counter using VHDL code becomes simpler because it is base on behavioural architecture in which to build these components, only descriptions of the properties of the input and output are needed without describing the structure in detail. In the design of frequency counter, there are two main components namely one-second time base and the counter block. To get a one-second time base, it was derived from the delay of 50,000,000 times from the clock frequency of 50 MHz which is available in the FPGA module. By using the time base, it can acquire the measurement data with the resolution of one hertz. By using a multiplexer, the frequency change of each sensor is transferred to the computer via serial communication successively.

The samples used in the experiment are kerosene, methanol, gasoline and alcohol contained in each sample bottle. The reference gas of nitrogen was flowed at 50 mL/min through the sample and sensor chamber as shown in Figure-3. The surface sensor will be drained by the nitrogen gas in the cleaning process by configuring to open the valve-1 and to close valve-2. The surface of the sensor will then be exposed with the vapor samples in the identification process by configuring to close valve-1 and to open valve-2. In the cleaning process, the frequency difference values are close to zero. While at the sampling process, the frequency difference will be large with negative or positive direction.

The identification process of sample vapor is described with the following procedures: nitrogen gas is flowed at a certain time until a frequency difference is stable. Change in the frequency difference is recorded in every second. At the time between 0 and 10 seconds, the nitrogen gases are flowed and then a vapor sample is discharged at between 11 and 130 seconds followed by nitrogen gas at between 131 and 250 seconds. Each sample was performed eight times to find the distribution of identification results and the reliability of the tool. The result of the data collection phase is 32 data sets for all samples. This data set has four dimensions as it is derived from the four sensors in the sensor array. The vapor pattern is taken from 30 data of the recorded data sets at the time between 80 and 110 seconds. Normalization of the data is desired to reduce a pattern variation due to variations in the vapor concentration. The normalized data is expressed by:

$$S_i^n = \frac{S_i}{S_{\max}}, \quad i = 0, 1, 2, 3 \quad (2)$$

where S_i is a sensor data set, S_{\max} is the highest value of the data set. The normalized data has a value in the range between 0 and 1. The whole data set is then analyzed to reduce the dimension of the data set using Principle Component Analysis (PCA). There are two sets of data that will be used to verify the classification performance using SVM classifiers including the unnormalized (Data-1) and the normalized (Data-2) data. In this study, the multi-class SVM classifier with a "one-against-one" was used because this approach is more accurate [13] [14] and faster in the training phase [15] [16]. Procedure classifiers "one-against-one" begins with [load data set] \rightarrow [split training / testing set] \rightarrow [create "one-against-one" models] \rightarrow [store binary classification and prediction] \rightarrow [classify using a "one-against-one" approach with polynomial kernel (train and test)] \rightarrow [display performance].

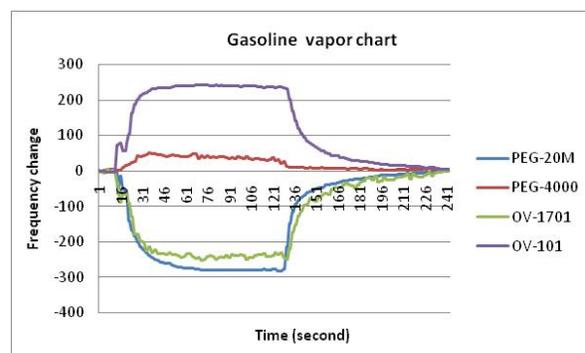


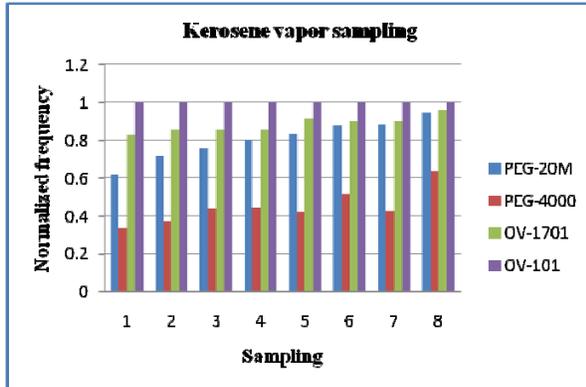
Figure-4. Sensor response to gasoline vapor.

RESULTS AND DISCUSSIONS

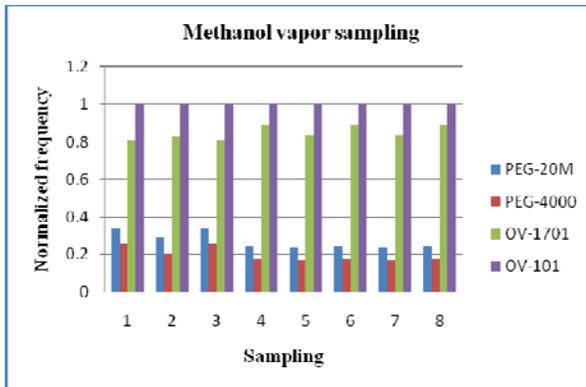
Figure-4 shows the sensor response exposed with gasoline vapor. The retrieval of 30 data, between 80 and



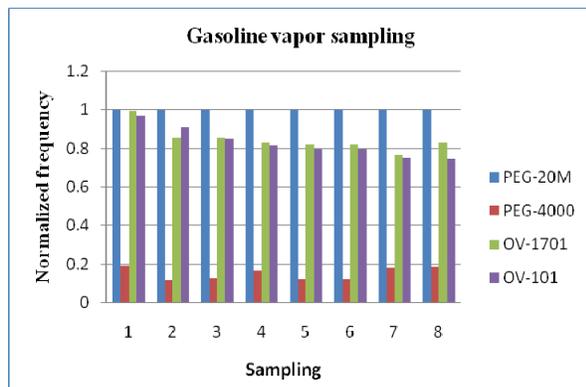
110 second shows that the condition of the sensor surface appears to have saturated with vapor molecules. Figure-5 shows the normalized pattern of four vapor samples obtained from the sensor response. The repetitive data for each sample shows that the each sample has the same pattern indicating the high reliability of the sensor response. The patterns of methanol and alcohol have a similar pattern due to its similar parameter of molecule polarity.



(a)



(b)



(c)

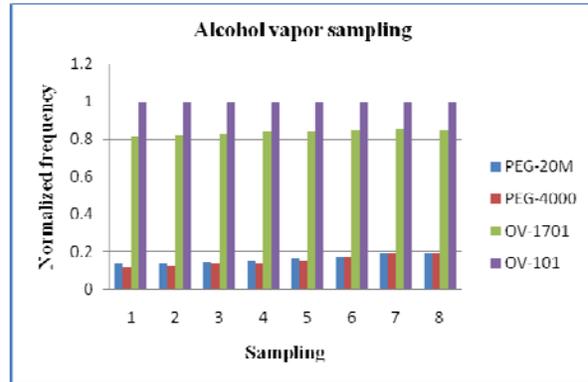


Figure-5. The pattern of sensor array to (a) kerosene, (b) methanol, (c) gasoline and (d) alcohol samples

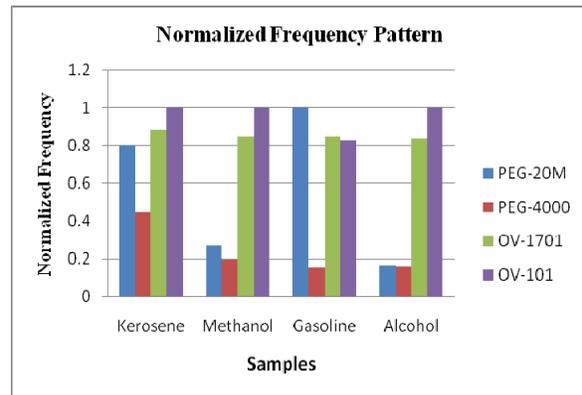


Figure-6. The normalized frequency shift.

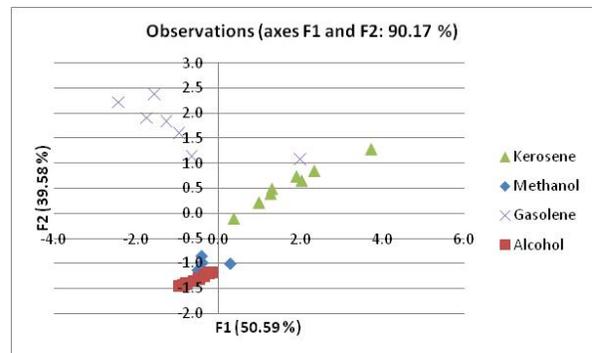


Figure-7. The scattering diagram provided by PCA.

The patterns of all samples are shown in Figure-6. Figure-7 describes a two-dimensional scatter plot to illustrate the distribution of data obtained from two principal components. The diagram indicates that the principal components of F1 and F2 could represent 90.17% variance of the data. The similar patterns of Methanol and Alcohol occupy most of locations in the scatter plot. Set of patterns of four samples can be distinguished from each other by using the SVM classifier involving a one-against-one with a 3rd degree polynomial



kernel in MATLAB. Classification results for the two data sets of Data-1 and Data-2 are shown in Figure-8. For unnormalized data set produces a classification with maximum accuracy rate of 97.2% having better performance than the normalized data sets.

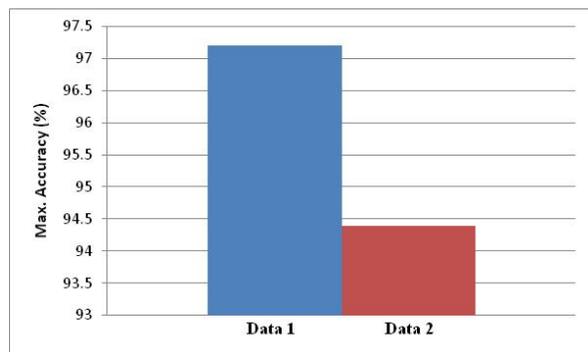


Figure-8. SVM classification performance.

The high variation of patterns will cause the projected data to spread in the scatter plot of PCA and to be more difficult in the classification stage.

CONCLUSIONS

In this study, it has been accomplished a vapor identification system using quartz resonator sensor array and support vector machine. PCA method was used to visualize the distribution of clustered data for each sample. It showed that the methanol and alcohol vapors have a similar location at the scatter plot indicating that the both molecules have similar physical properties. The SVM algorithm used in this experiment showed the high performance of classification achieving 97.2% and 94% for unnormalized and normalized data, respectively. For the future works, this method will be applied in the various applications including to examine the volatile organic compounds contained in exhaled human breath.

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