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Investigation of a Polymer-based SAW Sensor to Detect Volatile Organic Compound (VOC)

Nur Fatin Nabilah Mohamad Sabri, Nor F. Za'bah*, and Aliza Aini Md Ralib

Department of Electrical and Computer Engineering, Kulliyyah of Engineering, International Islamic University Malaysia, Kuala Lumpur

*Corresponding author: adah510@iium.edu.my

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Abstract— Two surface acoustic wave (SAW) sensors with polyethyleneimine (PEI) and polyisobutylene (PIB) layers respectively are modelled by using COMSOL Multiphysics software to detect acetone, benzene, and toluene. The main parameter of the SAW sensor is the thickness of the sensing layer, and the concentration of VOCs is varied to study their relationships with regard to the sensitivity of the SAW sensor. Both configurations portrayed the same pattern where the frequency shift and the sensitivity increase as the concentration of VOCs increases. In addition, the two layers have also produced promising results in sensing toluene even as low as 5 ppm which means that both layers are more selective towards toluene when the three VOCs are concurrently presented on the surface of the sensor. The data also shows that in detecting acetone and benzene, the PEI layer showed higher shifts in frequencies as compared to the PIB layer.

Keywords: *SAW sensor, Polymer, VOC*

1. INTRODUCTION

There has been a growing interest in investigating second and third hand smoke exposure. This is done by detecting the components in the smoke itself, particularly the volatile organic compounds (VOCs) such as acetone, benzene, and toluene. Second-hand smoke comes from tobacco that sticks on the cloth or hair during active smoking [1]. While third-hand smoke is the excess contamination from tobacco that remains after the cigarette has been put out [1].

Acetone, benzene, and toluene can be detected using commercially available sensors such as pellistor sensor [2]. The sensor detects VOCs by diffusing a mixture of air and VOCs through a porous sensor surface [4]. The porous sensor's main element is a coil made from platinum wire [2]. However, the main problem with this type of sensor is it needs to be heated up to hundreds of degrees by allowing the electric current to pass through the platinum wire [2]. Thus, this sensor is not suitable to be used at room temperature. Another type of sensor that can detect VOCs at room temperature is the SAW sensor, which uses a sensing layer such as metal oxides, polymers, and carbon nanotubes [1, 2]. However, in comparison with polymers, the sensitivity of metal oxides is low at room temperature, and they may exhibit a very long recovery time due to the involvement of redox reactions unlike polymers that generally absorb the gases via physisorption [2]. In addition, a SAW sensor with a metal oxide layer needs to operate at a high temperature environment to react with the gases [2]. Therefore, this paper will focus on simulating a SAW sensor using polymer as the sensing layer and its sensitivity and selectivity will be investigated by varying the relevant parameters such as the thickness of the polymer layer and the concentration of the VOCs.

1.1 SAW Sensor

Fig. 1 shows an illustration of a SAW sensor that includes an interdigital transducer (IDT), piezoelectric substrate and the sensing layer. In order to produce a SAW oscillator configuration, the sensor is connected in a high frequency amplifier feedback loop together with a phase compensation network [3]. The targeted analyte passes through an area between a pair of IDTs, a sensitive region covered with a sensing layer [4]. Once the analyte passes through the region, the sensing layer absorbs the targeted analyte which causes changes in elastic modulus, density, and thickness of the sensing layer [5]. The changes that occur to the sensing layer will change the acoustic wave velocity, which is measured in frequency shift [3, 6]. The frequency variation depends on the concentration

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of the targeted analyte. In addition, the targeted analyte also determines whether it is a positive frequency shift or a negative frequency shift. A positive frequency shift occurs because of mass loading while elastic loading causes a negative frequency shift [3].

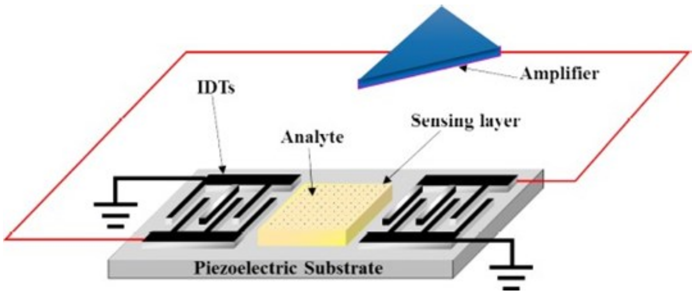

Fig. 1. An illustration of a SAW sensor detecting an analyte [3]

The frequency shift of the SAW oscillator because of mass loading can be calculated using Eq. (1) where k_1 and k_2 are constants of the piezoelectric substrate, h is the thickness of the sensing layer, f_0 is the unperturbed resonant frequency of SAW oscillator, Δm is mass loading and A is the area of sensing film [3, 7].

$$\Delta f = (k_1 + k_2)\, f_0^2\, (\Delta m/A) = (k_1 + k_2)\, f_0\, h\, k\, C_v \qquad (1)$$

The sensitivity of the SAW sensor towards the targeted analyte is also an important parameter to be investigated. In a SAW sensor, the sensitivity can be calculated using Eq. (2) where Δc is change of analyte concentration and can be expressed as Hz/ppm or Hz/vol [2, 8].

$$S = \frac{\Delta f}{\Delta c} \qquad (2)$$

2. METHODOLOGY

There are three main elements in designing a SAW sensor: the sensor's configuration, the piezoelectric substrate, and the sensing layer. There are two types of SAW sensors which are delay lines configuration and resonator configuration. Thus, this work uses the resonator configuration as it is more stable and produces less noise than the delay lines configuration. Secondly, YZ lithium niobate and ST-X quartz are widely used as piezoelectric substrates. This work proposed to use YZ lithium niobate as the material of piezoelectric substrate as it has higher wave velocity than ST-X quartz. Thirdly, the sensing layers that can be used with the sensor include polymer, metal oxides and carbon nanotubes. For this work, two types of polymers are used: polyethyleneimine (PEI) and polyisobutylene (PIB).

Next, the analytes that will be tested in this work are acetone, benzene, and toluene. These VOCs are the main components in second and third hand smoke.

2.1 Configuration in COMSOL

Fig.2 shows the detailed steps to model and simulate the SAW sensor using COMSOL Multiphysics software. Initially, the modelling of the VOCs requires five parameters which are:

i. concentration of the VOCs in ppm
ii. concentration of the VOCs in the air
iii. the molar mass of the VOCs (shown in Table 1)
iv. air partition constant for the VOCs in the polymers (shown in Table 1)
v. mass of concentration of the VOCs in the polymers.

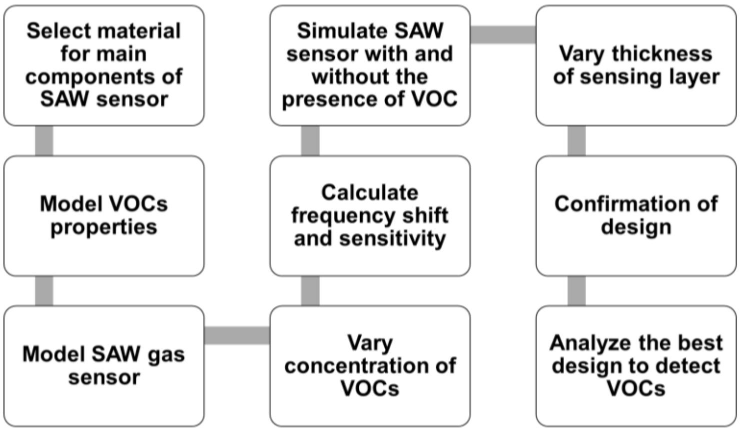

Fig. 2. The detailed step to model and simulate the SAW sensor with polymer as the sensing layer in COMSOL

Table 1: Some of the required parameters of VOC

Sensing Layer	VOCs	Molar mass (g/mol)	Air partition constant (K)
PEI	Acetone	58.08	1.15644
	Benzene	78.11	1.65549
	Toluene	92.14	2.06606
PIB	Acetone	58.08	1.20675
	Benzene	78.11	2.20792
	Toluene	92.14	2.75624

As the polymers were not listed in the library of materials in COMSOL Multiphysics software, the parameters of the polymers were filled in manually. The parameters needed for each polymer were Young's modulus, the Poisson's ratio, the density, and the polymer's relative permittivity, which are shown in Table 2.

Next, the SAW sensor was simulated without the presence of VOCs to obtain the resonance frequency. After that, the thickness of the polymers was varied along with the concentration of VOCs. In order to determine the best configurations to detect acetone, benzene and toluene, the frequency shift was calculated.

Table 2: Parameters of PEI and PIB to be configured in COMSOL

	PEI	**PIB**
Young's modulus (GPa)	3.04	10
Poisson's ratio	0.4008	0.48
Density (g/m^3)	1.27	0.918
Relative permittivity	3.3	2.2

Then, the proposed structure of the SAW sensor is shown in Table 3 and Fig. 3. From a single cigarette, approximately 50 ppm up to 550 ppm of acetone is produced, 10 ppm up to 60 ppm of benzene is generated and 5 ppm to 80 ppm of toluene is generated [9] which is the reason behind the VOCs concentration range.

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Table 3: The design of the SAW Sensor

Components	Description
Interdigital transducer	Material: Aluminum (Al)
Piezoelectric substrate	Material: YZ lithium niobate Acoustic wave velocity: 3960 m/s
Sensing element	1. **Polyethyleneimine (PEI)** The thickness of the sensing layer varied from 400 nm up to 600 nm. 2. **Polyisobutylene (PIB)** The thickness of the sensing layer varied from 200 nm up to 900 nm.
Volatile organic compounds concentration	1. **Acetone:** Concentration of acetone varied from 50 ppm up to 550 ppm. 2. **Benzene:** Concentration of benzene varied from 10 ppm up to 60 ppm. 3. **Toluene:** Concentration of toluene varied from 5 ppm up to 80 ppm.

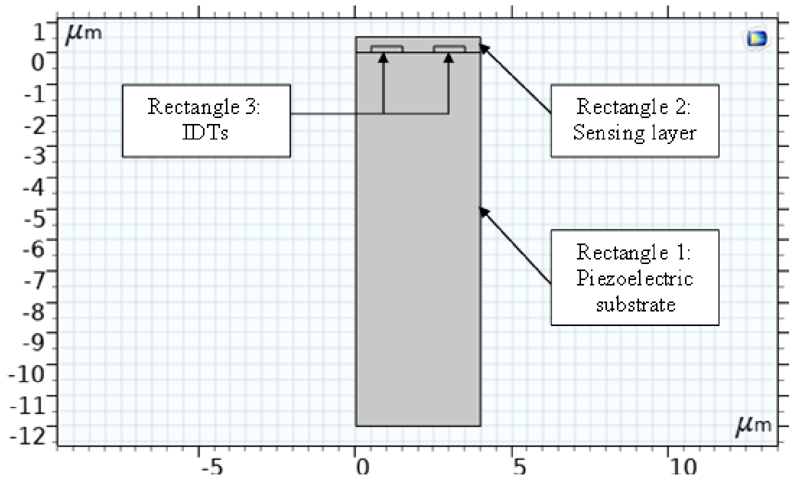

Fig. 3. Geometry of the SAW sensor that shows the interdigital transducer, the sensing layer and the piezoelectric substrate.

3. Result and Data Analysis

3.1 SAW sensor with Polyethyleneimine (PEI) as the Sensing Layer

In order to study the effect of the thickness of sensing layers, the thickness of the PEI layer was varied between 400 nm, 500 nm, and 600 nm. Fig. 4, Fig. 5, and Fig. 6 show the changes in the frequency shift when this SAW configuration is used to detect acetone, benzene, and toluene respectively. As can be seen from all these figures, there is a significant change in the frequency shift between 400 nm and 500 nm thickness. In addition, since there is not much difference between 500 nm and 600 nm, it can be concluded that the optimum thickness of PEI to be used as the sensing layer with the SAW sensor is 500 nm.

3.2 SAW sensor with Polyisobutylene (PIB) as the Sensing Layer

Next, as for PIB, the thickness of the PIB layer varied from 200 nm to 900 nm. However, by referring to Fig. 7, the frequency shift increased steadily. Thus, the optimum thickness of the PIB layer could not be determined.

3.3 Effect of Concentration of VOCs towards frequency shift and sensitivity

In order to know the sensitivity of the sensing layers to each of the VOC, the approach is to set the thickness of the polymers to 500 nm and to choose the same concentrations for each VOC which is 50 ppm. Next, using Eq. (2) to calculate the sensitivity of the SAW sensor.

The sets of data for PEI and PIB are shown in Fig. 8 and Fig. 9 respectively.

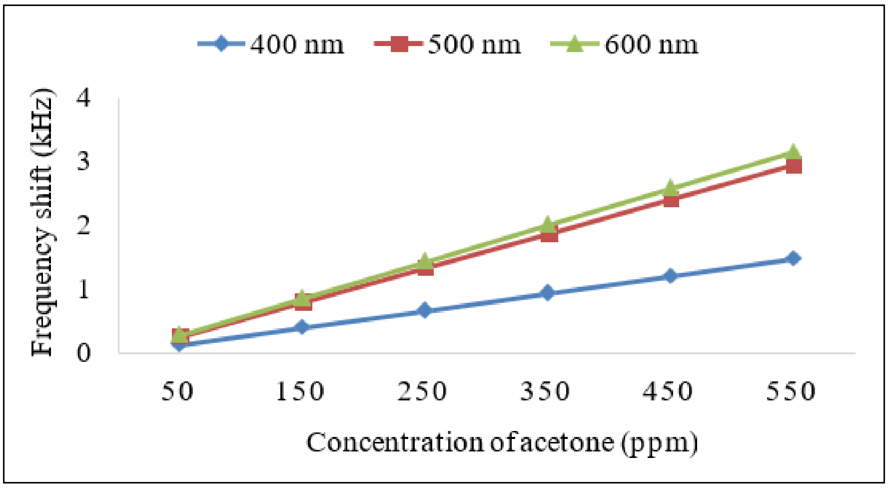

Fig. 4. SAW sensor with PEI sensing layer – detecting acetone

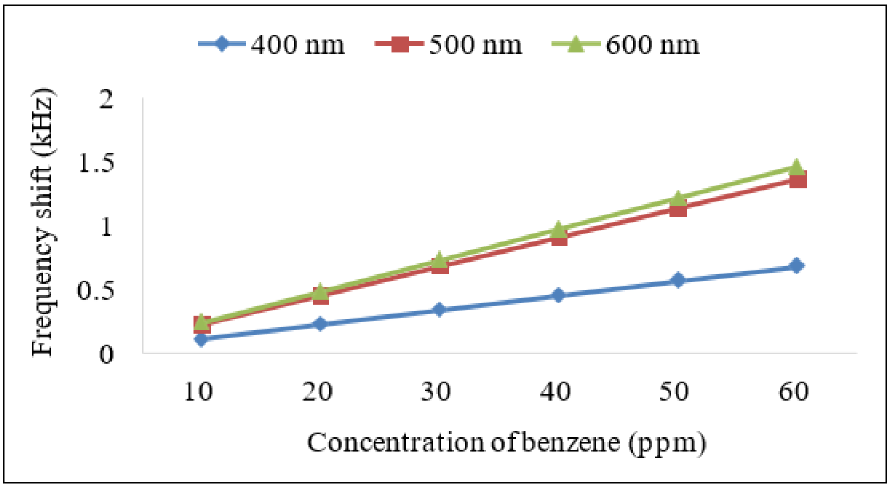

Fig. 5. SAW sensor with PEI sensing layer – detecting benzene

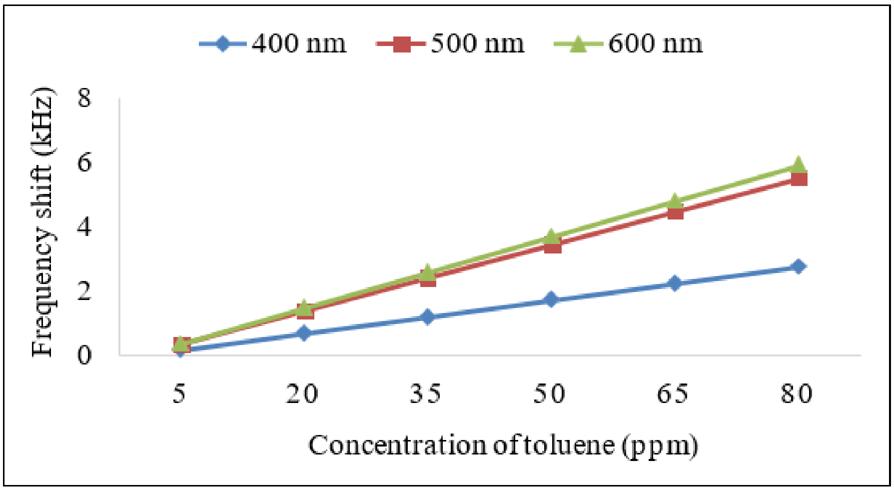

Fig. 6. SAW sensor with PEI sensing layer – detecting toluene

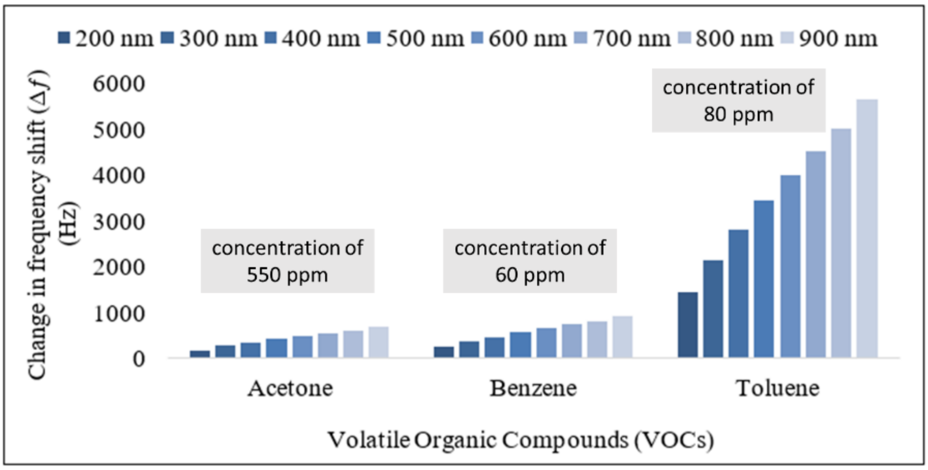

Fig. 7. Performance of PIB SAW sensor in sensing acetone, benzene, and toluene at specific concentrations.

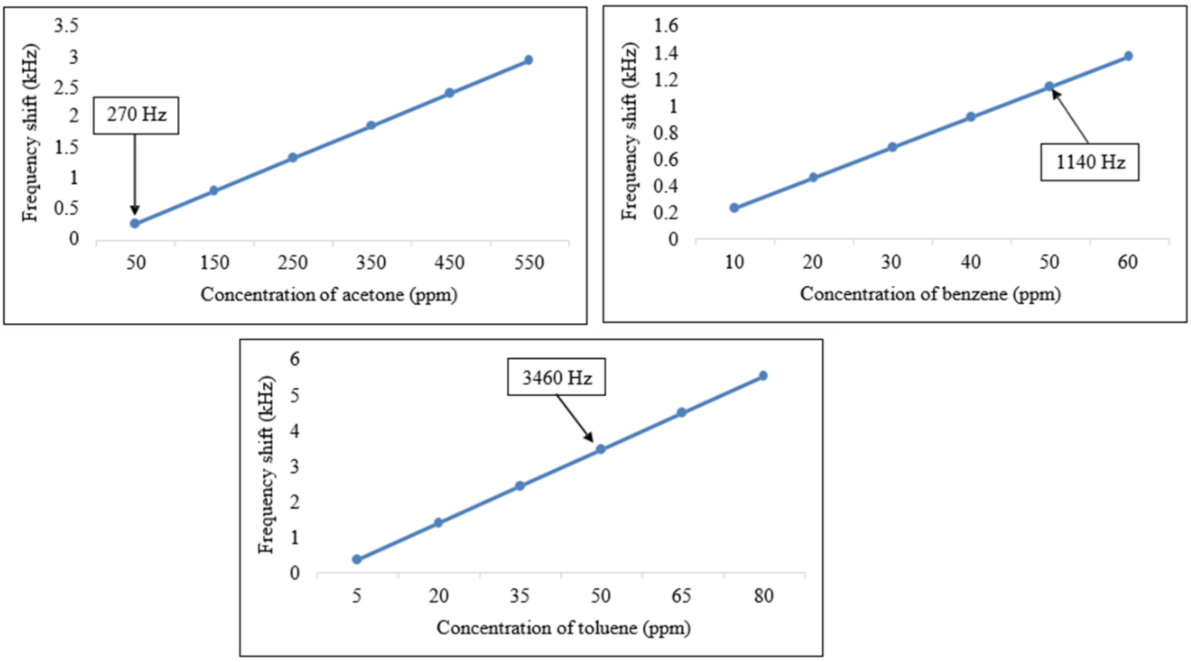

Fig. 8. The SAW sensor with PEI as the sensing element. The thickness of the PEI is set to 500 nm and the concentration of the VOCs is set to 50 ppm.

From these data, it can be concluded that PEI and PIB sensing layers are more sensitive towards toluene because the frequency shift caused by the presence of 50 ppm of toluene is the highest compared to acetone and benzene. Hence, it can also be assumed that both sensing layers will be more selective towards toluene when the three VOCs are presented on the surface of the sensor at the same time.

However, in comparison, for the detection of acetone and benzene, it can be observed that the PEI sensing layer is more suitable as it shows a much higher change in the frequency shift as compared to PIB.

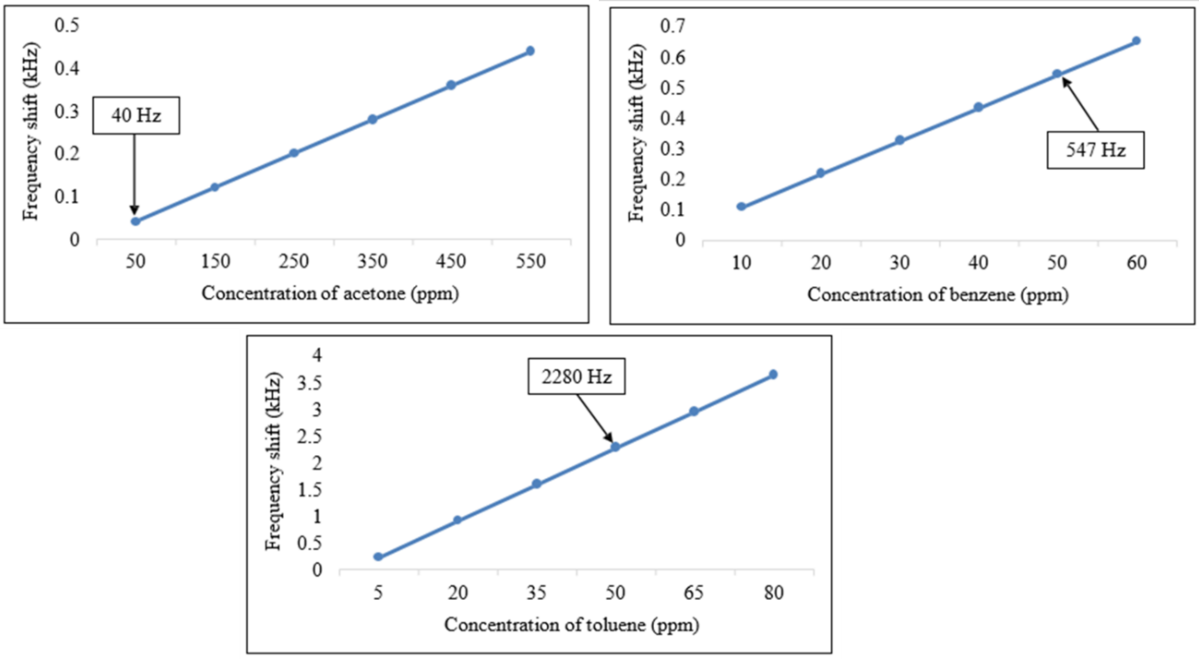

Fig. 9. The SAW sensor with PIB as the sensing element. The thickness of the PIB is set to 500 nm and the concentration of the VOCs is set to 50 ppm.

4. CONCLUSION

This work has presented a simulation of a polymer-based SAW sensor to detect acetone, benzene, and toluene. Two types of polymers were proposed as the sensing layers for the SAW sensor: polyethyleneimine (PEI) and polyisobutylene (PIB). Both configurations portrayed the same pattern where the frequency shift and sensitivity increase as the concentration of VOCs increases.

For PEI, the optimized thickness is 500 nm. Using the same thickness for PIB, the sensitivity of the sensors was investigated and both configurations produced promising results in sensing toluene even as low as 5 ppm. In detecting acetone and benzene, the PEI layer showed higher frequency shifts compared to the PIB layer.

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