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Modelling and simulation of micro pre-concentrator for pollution monitoring and explosive detection by trace level measurement of gas

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This paper presents the complete modeling of the pre-concentration cycle for the optimization of a micro gas pre-concentrator applied to atmospheric pollution monitoring[1]. If the concentration of dangerous gases for health like benzene and nitrobenzene are in the ppb (Parts per billion) level[2], and if not able to be detected by the gas sensor, then by using a pre-concentrator, the conversion of ppb level to ppm (Parts per million) level can be possible[3]. Hence, it can be easily detected by the gas sensors within a very short duration of time. Pre-concentrator is used for the improvement of the sensitivity of the gas sensor[4]. In the pre-concentrator with the use of adsorbent material for nitrobenzene and benzene gas, the accumulation of a measurable concentration of nitrobenzene gas or benzene gas on the porous Si as an adsorbent surface has been performed[5]. These molecules are then sending towards a detector (Gas Sensor) by desorbing it from the adsorbed surface. In this work, measurable concentrations of the gas are available in gas sensors which it can detect easily. The effect of the sensitivity of the device has been measured by varying the dimensions of the device. The simulation is done by COMSOL Multiphysics. The different designs and parameters (flow rate, heating cycle) have been investigated for performance optimization in terms of pre-concentrator factor and power consumption[6].

Keywords: Micro pre-concentration modeling, COMSOL Multiphysics, CFD module, adsorption, desorption, heat transfer module, gas sensor, benzene, nitrobenzene.

Introduction

In the present world, due to the increase in the huge amount of Industry in the cities, the problem of pollution has become a very serious concern. A pre-concentrator is a device that is used with a gas detector to bring a very less concentration (unmeasurable concentration) of target gas into a measurable concentration range of the detector. Benzene and nitrobenzene is a toxic gas[7]. It's a very small concentration presence in an atmosphere and is dangerous for the health of the human are difficult to detect by the gas sensor. So we accumulate the gases by pre-concentrator then a measurable quantity of gases is sent towards detector. We are working on the designing of the pre-concentrator in such a way so that maximum adsorption takes place at adsorbent surface and uniform desorption takes place at heater then it sends towards the detector. Since pre-concentrator has become useful in increasing the selectivity and sensitivity of the detection[8] (an example in the field of the health sector), hence it can monitor the health of the patients just by measuring the gas molecules present in the exhaled air by the patient[9].

Working method

In the pre-concentrator with the use of adsorbent material we accumulate a measurable concentration of gas molecules on an adorable surface, and then these molecules send towards a detector by desorbing it from the absorbable surface. In this way we detect the presence of very low concentration gas. So we are modelling the pre-concentrator by varying the shape of the channel, shape of the heater by CFD (Computational Fluid Dynamics) module for the improvement of the sensitivity of the device[10].

Modeling process

Modelling of pre-concentrator is done by COMSOL Multiphysics software in which CFD (Computational Fluid

Dynamics) module is used[11]. Here, the design of the channel is such a way that maximum adsorption will take place. So for maximum adsorption, the pressure gradient at the adsorbent surface should be high and the velocity gradient should be low, and uniform[12]. The process of simulation has been explained in the next sections.

Simulation process:

In this design, micro channels, based on porous silicon substrate filled with the paste of Tenax TA polymer are implemented for selective adsorption of nitrobenzene at low temperature and micro channels, based on porous silicon subtract filled with SWCNT (Single Wall Carbon Nano Tubes) are implemented for selective adsorption of benzene gas at low temperature[13]. SWCNT is selected as an adsorbent material due to its high surface area, low affinity with water, good affinity towards benzene gas molecules, and moderate desorption temperature[14]. Tenax-TA polymer is selected as an adsorbent material due to its large adsorption capacity with nitrobenzene molecules, and low activation energy of desorption at a temperature below 150°C. The desorption peak amplitude for this polymer as an absorbent material has obtained at 120°C. Porous Si substrate which is used to increase the gravity of adsorbent filled in micro channel. Compared to non-porous silicon, it also increases the good binding of particles to avoid an evacuation or the deposition under high gas flows[15]. The CFD module is used for designing of channel and heater which is described below.

COMSOL Multiphysics (CFD Module) for modelling of channel:

In this work, the study of the velocity and pressure gradient of gases under different shapes of the channel for a particular absorbent has been done. Also, the analysis of how to get uniform velocity throughout the channel, and maximum pressure gradient in that respective channel where the heater is connected has been carried out.

COMSOL Multiphysics (Heat Transfer Module) for modelling of heater:

The design of a heater that can be integrated on the backside of the silicon substrate by the use of screen printing having a high melting point is performed. This can provide the desired temperature for adsorption and desorption up to 500°C with low resistivity. Hence, the heater will provide a very homogeneous distribution of temperature with low heat interface stress so that heat loss can be less.

Types of materials used in making of pre-concentrator

There are two types of material used in the making of pre-concentrator. These are explained briefly below.

Subtract type:

Here, a porous silicon substrate is used instead of a normal silicon substrate as it can give maximum adsorption and getting desorption peak intensity at very low temperature as compared to non-porous silicon substrate shown in Fig. 1.

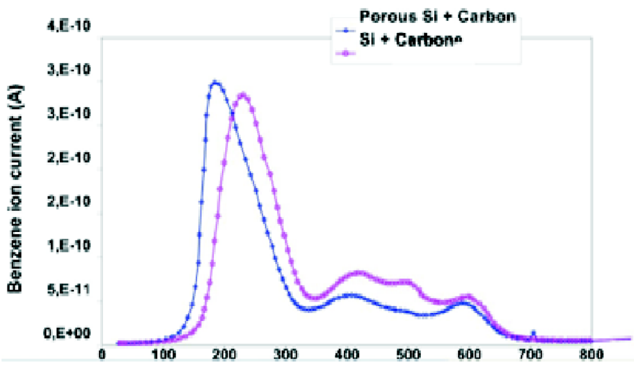

Fig. 1. Porous vs non-porous[1].

Hence, porous Si subtract has used for this modeling.

Adsorbent type:

There are so many absorbent available for different gases which have to detect first. The absorbents need to have properties like large adsorption capacity of the target gas, affinity with a target gas should be very high, and particles should bind with the substrate of pre-concentrator tightly so that its particles do not evacuate from the substrate during the flow of high gases. These available absorbents are used for benzene and nitrobenzene gases[16].

Carbon nano powder as an adsorbent:

It can be used as an adsorbent material for the benzene gas because it has a good binding with benzene gas molecules. The surface area of carbon nano powder is 99 (m^2/g) and its particle size is 0.1 um. The thermally activated carbon nano powder surface area is up to 490 (m^2/g)[17].

Drawback: Carbon nano powder does not prove as an idle adsorbent for the benzene gas molecules because the effect of humidity at carbon nano powder is much high (Fig. 2). So at the time of desorption of benzene gas molecules from the surface of carbon nano powder, there will be a significant part of the current peak due to water vapor molecules[18].

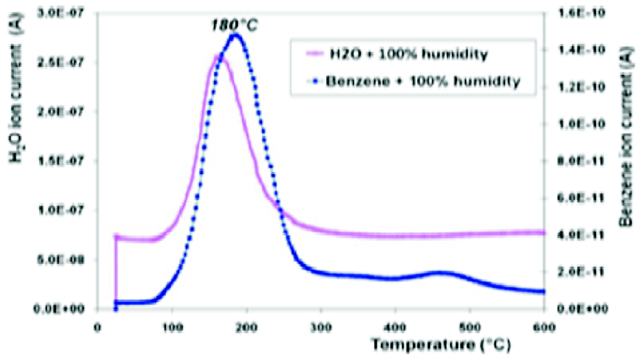

Fig. 2. TPD spectrum for carbon nano powder[17].

So carbon nano powder is not used as an adsorbent for benzene and nitrobenzene.

Multiwall Carbon Nano Tube (MWCNT) as an adsorbent:

It is a cylindrical hollow nano structure of the graphene sheet. The surface area of multi wall carbon nano tube (MWCNT) is 21 (m^2/g) and particle size is 5 (µm)[18].

Drawback: Requires a very high desorption temperature (480°C approx.) for benzene gas molecules. The effect of water vapour molecules on the multiwall carbon nano tube surface is very much high.

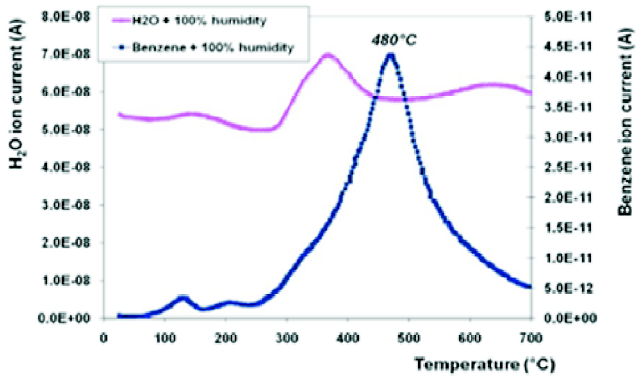

Fig. 3. TPD (Temperature Programmed Desorption) spectrum of MWCNT[13].

Hence the multiwall carbon nanotube is not used as an adsorbent in both benzene and nitrobenzene gases.

Tenax-TA polymer as an adsorbent for benzene gases:

It is a porous polymer resin based on 2,6-diphenylene oxide. Its surface area is 35 (m^2/g) and its particle size is 250 (µm). It has a low intermolecular binding force with benzene gas molecules.

Drawback: The effect of humidity is good. So the current peak due to water vapour molecules is significant.

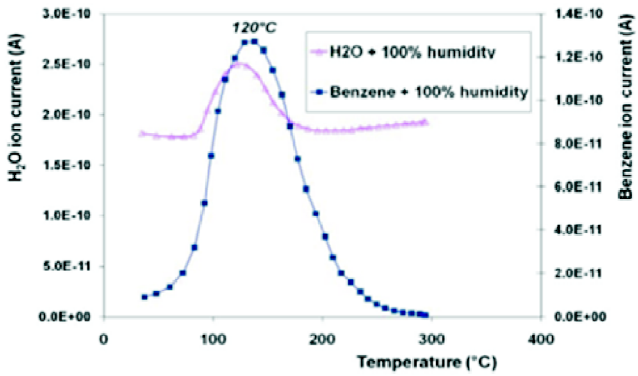

Fig. 4. TPD spectrum of Tenax-TA[16].

So it is not preferred as an adsorbent for benzene gas.

Tenax-TA (Thermal Analysis) polymer as an absorbent for nitrobenzene gases:

In this process, the adsorption peak intensity at very low temperature (120°C) has obtained and the effect of moisture will not affect the adsorption for nitrobenzene gas (Fig. 5). But this will not hold for benzene gas, as the intensity peak is very low even at very high temperatures. That's why, Tenax-TA polymer is used for nitrobenzene, and not for benzene.

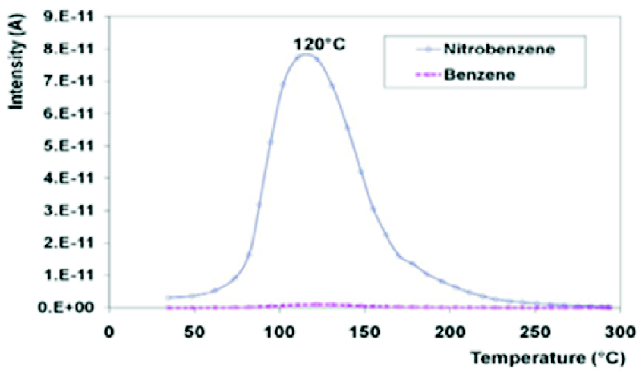

Fig. 5. TPD for benzene and nitrobenzene.

Hence it is recommended to use Tenax-TA (Thermal Analysis) polymer for the adsorbent for nitrobenzene gases.

Single Wall Carbon Nano Tube (SWCNT) as an absorbent for benzene:

It is a single layer hollow cylindrical structure of grapheme sheet. Its surface area is 400 (m^2/g) approx. and its particle size is 2 (μm).

Advantage: Its surface area is very high. The requirement of moderate activation energy (desorption temperature, near about 260°C approx.) and the effect of water vapour molecules on the surface of single wall carbon nano tube (SWCNT) is least (very low as compare to the other adsorbent).

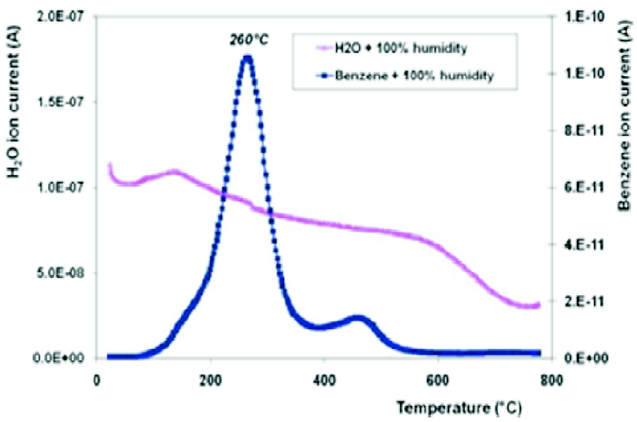

Fig. 6. TPD spectrum for SWCNT[18].

So SWCNT is used as an adsorbent for benzene gases.

Design of channel

In micro pre-concentrator, there is a requirement of the channel through which the target gas will pass. In this channel, adsorption and desorption mechanism will take place. For the formation of channel in the porous Si substrate, a deep reactive ion etching process is used. In this method, the wafer is chilled to –110°C and ions are bombarded on the upward-facing surface of the wafer. As a result of this etching of wafer will take place. So the design of the channel should be in such a way that the maximum adsorption of the target gas on the surface of the channel will take place. So it can easily able to give an activation energy to the channel with the help of heater for desorption. There are many design of channels is available. One of them is the V-shaped channel. In this design of channel, when target gas enters from the inlet and comes out from the outlet, the maximum adsorption can take place due to this V-shaped structure. But the sudden change in geometry may cause pressure loss which is not desirable. Also in this design, the integration of the heater on the backside of the channel is not easy. Hence, this design of the pre-concentrator channel has some limitations.

Zigzag channel:

In this design, due to the zigzag path of the channel, the adsorption of target gas on the surface of adsorbent will maximum. The target gas interaction with the inner wall of the channel is high; hence the adsorption will be more. But due to the sudden bending of the channel in it, the pressure loss will be more which is not good for the performance of the pre-concentrator[19]. Due to the zigzag path, the integration of the heater on the backside of the channel in this design is also difficult for providing thermal energy to the channel. Hence it has also some limitations.

Square and curve shaped channel:

The modelling of different shapes of square and curved shaped channel is needed. Also the analysis of velocity and pressure gradient of gases, and study of the adsorption phenomenon is carried out further.

Velocity gradient and pressure gradient for benzene and nitro-benzene gases

Different shaped channel (Square shaped and curved shaved) by using several attempts with passing gas having inlet velocity 0.2 m/s is used here. After meshing, the study of velocity and pressure gradient for each different shaped channel is done. For the good adsorption, the velocity gradient should be low and uniform and the pressure gradient should be high after adsorption.

Result of simulation for benzene and nitrobenzene gas by CFD soft-ware modules for different shaped channels

After the meshing, different results will be obtained (Figs. 7 and 8). These figures can easily describe the velocity and pressure gradient.

Velocity gradient for benzene gas by CFD software analysis for square shaped channel:

When the benzene gas is passed in the square box geometry of channel by giving an inlet velocity (0.2 m/s), it has observed that the velocity of benzene gas throughout the channel remained constant except a very little variation at the top surface of the channel wall. For the maximum adsorption on the surface of the channel wall, velocity should be moderate. It should not be so much high or so much low rather should be moderate at the given inlet velocity. It has found that in a square box, the geometry velocity remains almost the same at every slice of the square box and is equal to the inlet velocity. Hence square box geometry of the channel is good channel geometry for the maximum adsorption of the channel wall.

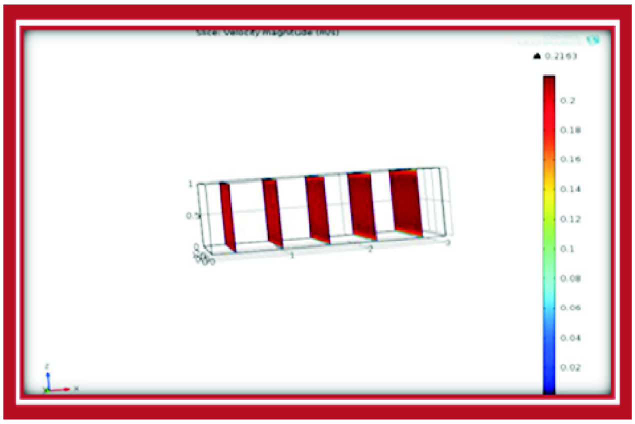

Fig. 7. Velocity gradient for square channel obtained from the CFD module.

Pressure gradient for benzene gas by CFD software analysis for square shaped channel:

For the maximum adsorption of benzene gas on the surface of the channel wall, the pressure exerted by it on the channel wall should be very high. In the analysis, it is seen that, in the square box geometry of the channel, the pressure exerted by the benzene gas on the inner wall of the channel is very low. So it is not a sufficient condition for the maximum adsorption of the benzene gas on the surface of the adsorbent. After analysing the pressure and velocity graph of benzene gas in the square box geometry of the micro pre-concentrator channel, it can be concluded that this square box geometry is good but not an idle geometry for micro pre-concentrator because of low pressure.

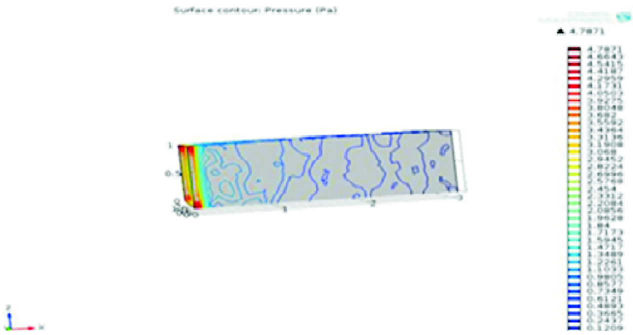

Fig. 8. Pressure gradient for square channel obtained from the CFD module.

Pressure gradient for benzene gas by CFD module analysis for curved shape channel:

The benzene gas has passed inside the curved shape geometry of the micro pre-concentrator channel and analysis of the pressure exerted by the benzene gas on the inner wall of the micro pre-concentrator channel is carried out, we have found that in curved shape geometry of micro pre-concentrator channel, the pressure exerted by it on the inner wall of the channel is good which is required for the maximum adsorption of the benzene gas on the adsorbent surface. Hence curved shape geometry of the micro pre-concentrator channel is good.

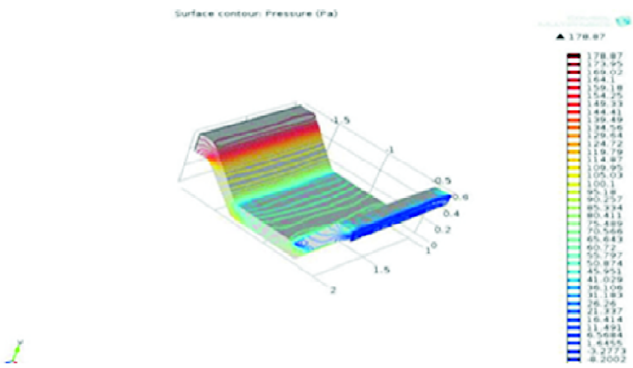

Fig. 9. Pressure gradient for curved surface obtained from the CFD module.

Velocity gradient for benzene gas by CFD module analysis for curved shape channel:

From Fig. 10, it is clear that the velocity gradient across the center of the curved surface is uniform and low.

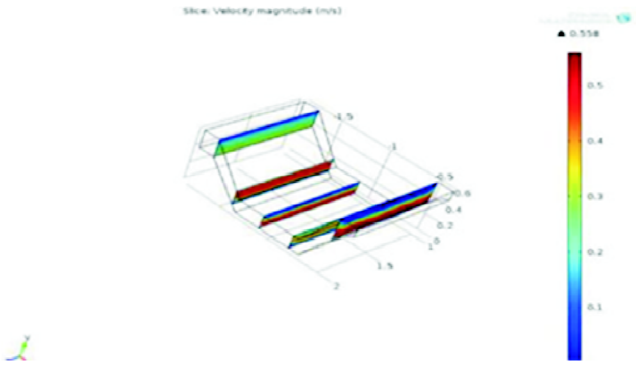

Fig. 10. Variation in velocity of benzene gas in Curved-1 geometry of channel obtained from the CFD module.

Hence, it can be said that the curved shape geometry of the pre-concentrator channel will be better geometry for the micro pre-concentrator channel as compared to square type.

Pressure gradient for nitrobenzene gas by CFD module analysis for curved shape channel:

Pressure gradient is high and uniform across the horizontal surface area as shown in Fig. 11.

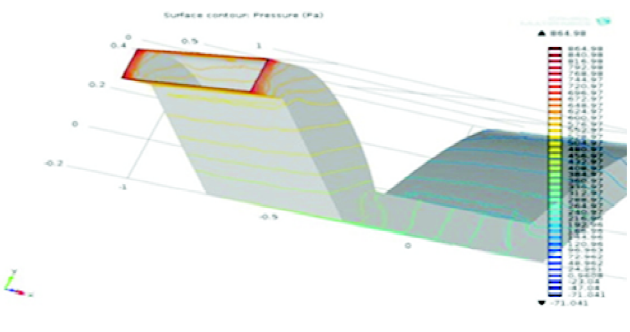

Fig. 11. Pressure gradient for nitrobenzene gas obtained from the CFD module.

Velocity gradient for nitrobenzene gas by CFD module analysis for curved shape channel:

Velocity is constant along the middle of channel and pressure is high across the channel and remains constant through horizontal surface where the heater is connected so curved surface is better for nitrobenzene also.

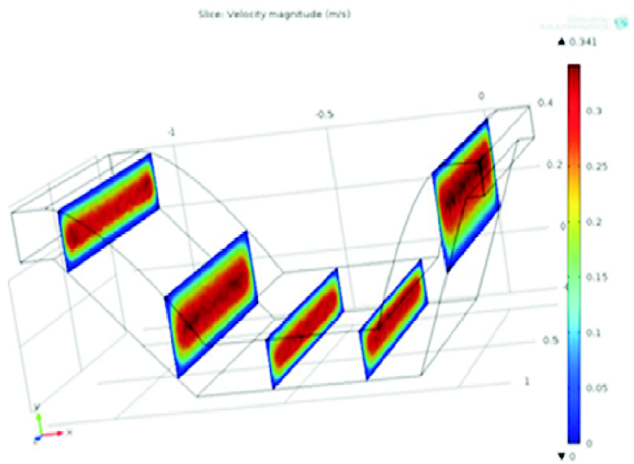

Fig. 12. velocity gradient of nitrobenzene for curved surface obtained from the CFD module.

Result for simulation of benzene and nitrobenzene gas by CFD software modules for designing of heater

The uniform heating is required so that uniform desorption can take place and hence, the accumulated gas can be sent towards the detector.

Design of heater:

After the adsorption in the absorbent material like SWCNT for benzene and Tenax-TA polymer for nitrobenzene, a heater is required for desorbing absorbent gases (benzene, nitrogen). The heater design should be done through the CFD module in such a way that material should have a high melting point and uniform temperature distribution[20].

Study of nichrome wire heater by CFD module software:

During the simulation of nichrome wire heater, when a 12 V battery is connected with a heater wire, its potential decrease in nichrome wire slowly with respect to distance (Fig. 13). This is because the resistivity of a nichrome wires is very low (0.00000110 Ω m to 0.00000150 Ω m).

Nichrome heater temperature study by CFD module:

From the above figure, it is concluded that this design of nichrome heater temperature is uniformly distributed to the entire heater and having a temperature of 420°C without melting the heater.

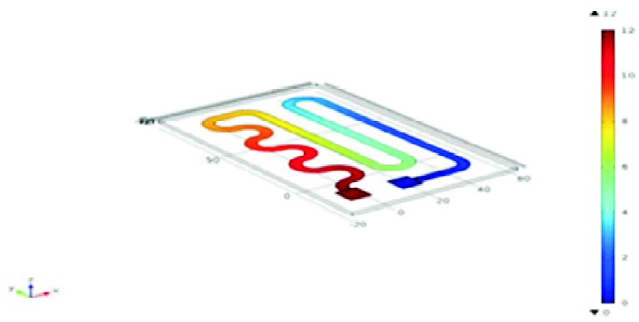

Fig. 13. Voltage gradient for nichrome wire obtained from the CFD module.

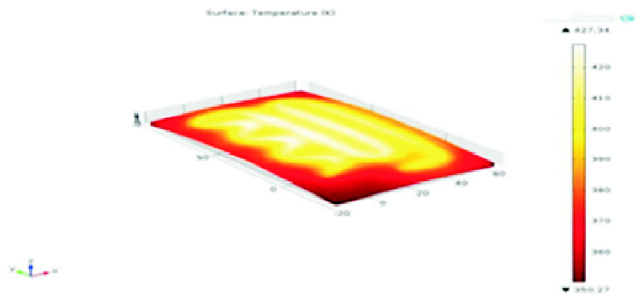

Fig. 14. Temperature distribution across the nichrome heater obtained from the CFD module.

Nichrome heater interface stress:

The interface stress generated by the heater to the subtract is uniform and less as shown in Fig. 15.

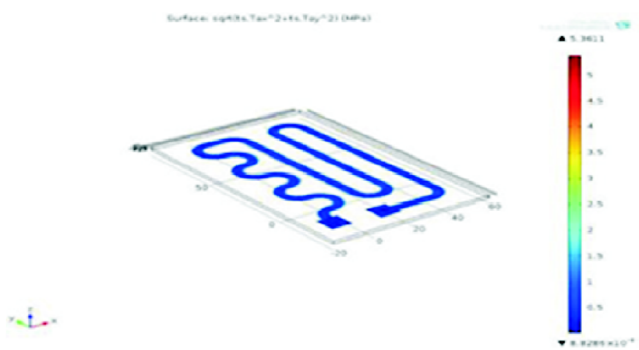

Fig. 15. Interface stress distribution obtained from the CFD module.

Nichrome heater stress Top:

It can be seen that only at the bending, the stress is significant, but in the rest of the other places, stress is less so that there will be loss of energy only at a bending and in other places, there will be no loss of energy.

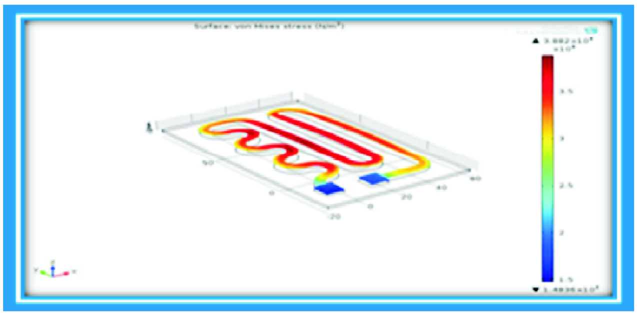

Fig. 16. Stress distribution across bending obtained from CFD module.

Experimental analyses

In this work, all the experiments have been performed in the experimental lab CSIO (Central Scientific Instruments Organisation), Chandigarh, India which is a national laboratory dedicated to research, design, and development of scientific and industrial instruments. By observing the behaviour of silicon substrate along with the adsorbent material SWCNT on its surface at different temperatures in the presence of air, it is found that at 24°C, the deflection in current with respect to voltage is very high. So it can be said that, Si substrate along with SWCNT has the highest adsorption capacity for the air at 24°C.

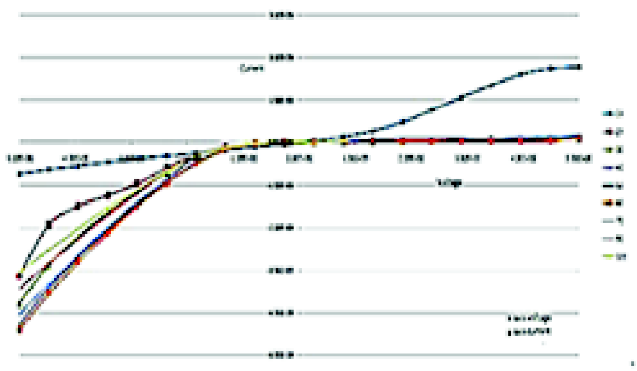

Fig. 17. I-V Characteristics of Si substrate with SWCNT as an adsorbent in the presence of air.

After the analysis of silicon substrate along with adsorbent material SWCNT on its surface, in presence of benzene gas, it is found that there is the maximum variation in I-V characteristics of the silicon substrate having that adsorbent material in the presence of benzene at 40°C. Hence, it can be stated that Si substrate and the absorbent has a maximum adsorption capacity for benzene gas at temperature 40°C. So in micro pre-concentrator, a temperature of 40°C should be kept so that maximum adsorption of benzene molecule on the adsorbent surface will take place.

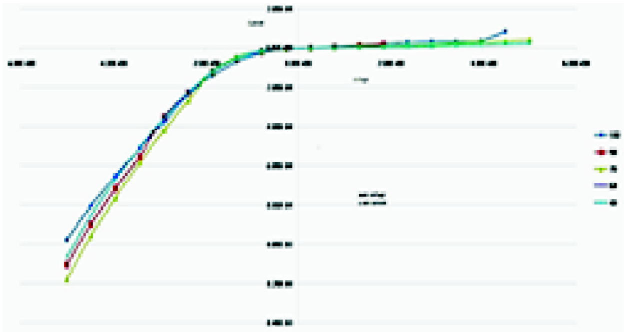

Fig. 18. I-V Characteristics of Si substrate with SWCNT as adsorbent in presence of benzene gas.

Conclusion

After the completion of the entire process, it is found that a curved shaped channel will be suitable for maximum adsorption across the channel for the pre-concentrator of gas. This is because it can give maximum adsorption of a gas as compared to the square box design of the channel due to its less and uniform velocity gradient, and high-pressure gradient. In the case of heating element, a nichrome heater will be suitable for our device due to its low resistivity, higher boiling point, and low cost, uniform heat distribution. The shape of the heater is as per study through COMSOL (Fig. 13, Fig. 14 and Fig. 15) which creates the least heat lost and uniform temperature across the channel. For adsorbent material, SWCNT is best for benzene gas due to its moderate temperature and less affected with humidity. Similarly, Tenax-TA polymer is the best adsorbent material for nitrobenzene gas as it will give maximum adsorption peak at low temperature 120°C with less effective to humidity. Again, it is difficult to design a pre-concentrator in micro-level size manually. So software can be used in modelling. The novelty of this work is its implementation through COMSOL Multiphysics software. Design of subtract and heater are unique.

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