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Modelling of a GC based Pre-Concentrator Covering Material for SAW E-Nose Gas Sensor

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ABSTRACT

This paper presents a modelling cum flexibility study to aid in the development of a Gas Chromatograph (GC) based pre-concentrator technology for Surface Acoustic Wave (SAW) sensor applications. Finite Element Method is computationally adopted and implemented via commercially available software COMSOL Multiphysics. A pre-concentrator device has been modelled, simulated with different covering materials and studied by cyclic micro heating and cooling of the Nichrome heating element for the purpose of device temperature stability. A temperature profile for two materials (Teflon with Aluminum and Teflon without Aluminum) as covering material of pre-concentrator is studied and the conclusions from such a study are reported.

Keywords: COMSOL multiphysics; Gas chromatography; Joule heating; Preconcentrator; SAW sensor.

1. INTRODUCTION

In the present age, explosive scientific and technological advancements in industrialization and terrorism are the main cause of environmental pollution, public safety and security. Gas phase chemical sensors plays a vital role in environmental monitoring, defence and internal security sector (Subramanian Sankaranarayanan *et al.* 2005; Sakairi, 2008). In many applications, the sensor and data collection and processing must be distributed and placed in inhospitable or inaccessible environments. To facilitate sensing in such environments, the sensor system must be self- contained and preferably accessed using wireless communication techniques. Designing reliable, cost effective, and small sized wireless sensors poses significant challenges to the scientific community (Haresh M. Pandya *et al.* 2011a). In order to that, such scenarios vapor sensors of high sensitivity and ability to differentiate the chemical and biological species is necessary. Therefore, the development of smart sensors for distributed measurement and control capability can be very useful to the energy industries, military and other industrial organizations (Haresh M. Pandya *et al.* 2011b; Datta, 1986).

Trace detection of Chemical Warfare Agents (CWAs), Toxic Industrial Chemicals and Materials (TICs/TIMs) andvolatile organic compounds (VOCs) is an important issue for any analytical system involved in military and other industrial applications. The scientific and technological advancement are required and suitable devices such as smart sensors are needed in the defence and internal security sector for reliable and timely detection of these toxic and harmful gases/vapors to preserve the invaluable human life and property. In order to detect in such scenarios vapour sensors of high sensitivity and ability to differentiate the chemical species is necessary. There are various types of vapour sensing techniques for trace level detection of these vapours, such as Ion Mobility Spectrometry (IMS), Flame Photometry, Surface Acoustic Wave (SAW) Electronic Nose and Chemo-Resistor Electronic Nose.

Surface Acoustic Wave (SAW) based sensors are one of the preferable technology for the detection of chemical warfare agents because of their high sensitivity irrespective of temperature, short time response, low power consumption, wireless detection, miniaturized size and low cost. Hence, great deals of research efforts arerequired towards the development of efficient sensing devices such as electronic nose (e-Nose) for timely detection of Chemical Warfare Agents (CWAs).A SAW e-Nose (fig. 1) is a chemical vapor sensor which mimics the human nose in smell recognition SAW electronic noses are realized with SAW devices as sensors in conjunction with Gas Chromatography (GC) followed by Pattern Recognition (PR) (Haresh M. Pandya *et al.* 2013). The Surface Acoustic Wave (SAW) electronic Nose is a versatile chemical vapour detector handheld equipment, capable of detecting vapour levels down to few parts per billion (ppb), in field conditions.

In SAW e-Nose, a Preconcentrator tube with a gas chromatograph (GC) column placed in front of the SAW device can improve its noise to signal ratio (SNR) and lower its detection limit. Pre-concentration is performed by collecting an analyte over a period of time and then, through a thermal heat pulse applied to the Preconcentrator, the collected analytes are released as a concentrated wave into gas chromatograph (Taiyo Yuden Navigator). A GC separates the mixture of vapors over time, a SAW sensor senses the vapors followed by electronics. The output is in the form of Gas Chromatogram, shift in frequency versus time, as shown in the figure where various peaks correspond to the various gases in a mixture.

A preconcentrator in a micro analytical system, which extracts the target analytes from the sample matrix, concentrates them, and injects them into the separation column (GC)) (Venkatesan and Haresh M. Pandya, 2013). In some cases, temporal separation of vapor mixtures can be obtained by the Preconcentrator as different compounds desorb at different rates. In such cases, the Preconcentrator is coupled directly with the gas sensor with no need of the chromatographic column. Park and Zellers demonstrated quantitatively (Haresh M. Pandya, 2015), using a porous styrenedivinylbenzene copolymer adsorbent in combination with a SAW sensor array, that the tested vapors desorbed after the initial humidity spike and were independent of the sampled humidity. Two main preconcentration methods are mostly used when dealing with gas-phase samples such as cryogenic or sorption trapping. The word "sorption" is used as a general term for indicating adsorption and absorption, which could take place simultaneously. Trapping by cryogenic condensation is done by passing the sample through a cooled narrow glass tube, usually filled with carbonaceous materials such as activated Carbon granules (Haresh M. Pandya, 2010). For a SAW E-Nose, cryogenic preconcentration is only possible in combination with sorbent agents. However, covering or shielding the Preconcentrator tube with the help of heat sink is necessary to enhance the thermal stability and power management of the device (Williamson, 1977; Sharma *et al.* 1973; Baranowski *et al.* 1971).

In our present work, a pre-concentrator device has been modelled through finite element modelling (FEM) approach, which is used in SAW E- Nose with the aim of improving their performance by refreshing SAW active area by successive heating and cooling. The main objective of our work is to achieve low power consumption and a uniform temperature distribution (350K-450K) over the adsorbent material region which is the working temperature targeted for our gas sensor platform. The analysis results suggest that the working power should be around 5 watts. More work is being done to calculate the power consumption with the simulation results. The simulation will also allow us to verify the efficiency of the current design and will suggest if any modification is needed.

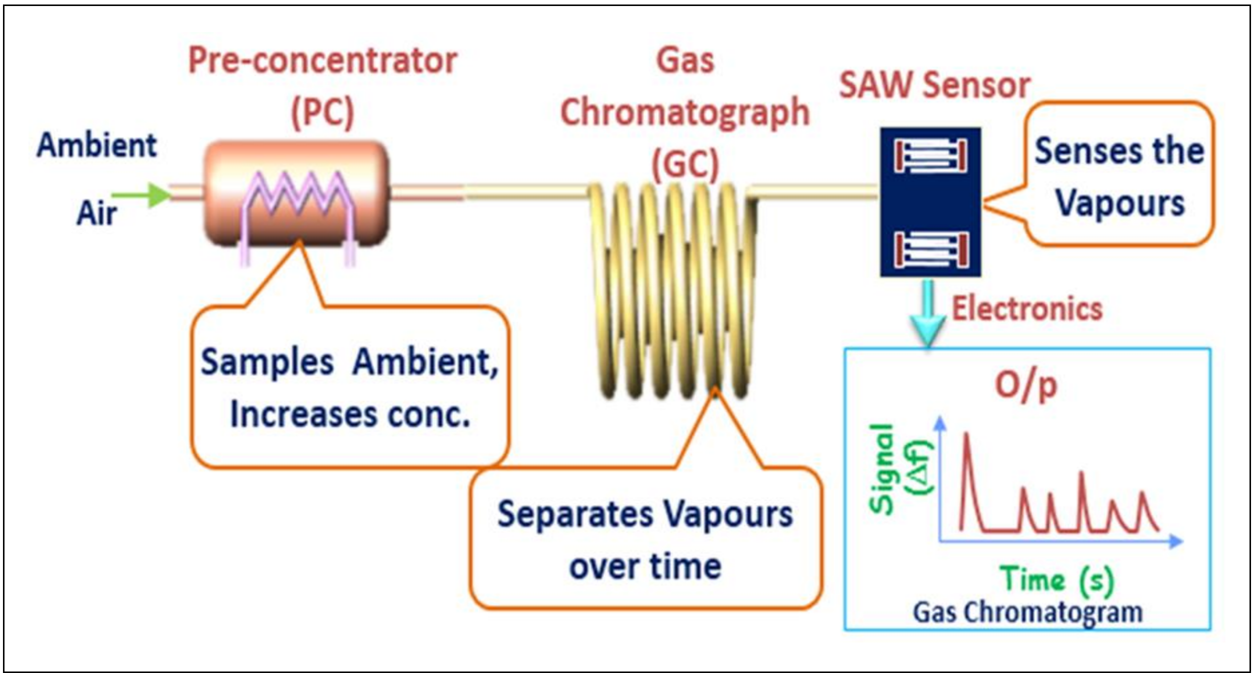

Fig. 1: Schematic of SAW e-nose

Fig. 2: Commercial thermal desorption preconcentration tubes (William B. J. Zimmerman, 2006)

2. SIMULATION SETUP

A 3-dimensional Finite Element Method (FEM) is used to estimate the temperature distribution on the device. COMSOL Multiphysics is the software which has been chosen to model and stimulate the device. All FEM models were performed on a sophisticated Intel core i7 computer system with 8GB RAM.A thermal-electric coupled field analysis was also performed to observe the heat release and heat distribution of the Preconcentrator tube as electric power is applied. Fig. 1 shows the model of the Preconcentrator tube used for this analysis.

The total size of the deviceis (7 mm × 7 mm × 5 cm). Nichrome wire is used as heat source and activated Carbon granules are employed as adsorbent material. Teflon alone and Teflon with Aluminium are used to cover the pre-concentrator. Initially 2D geometry is selected first during the simulation and then is extended to include 3D geometry also. The device dimensions (fig. 3) and the material parameters of 3D module is given in table 1.

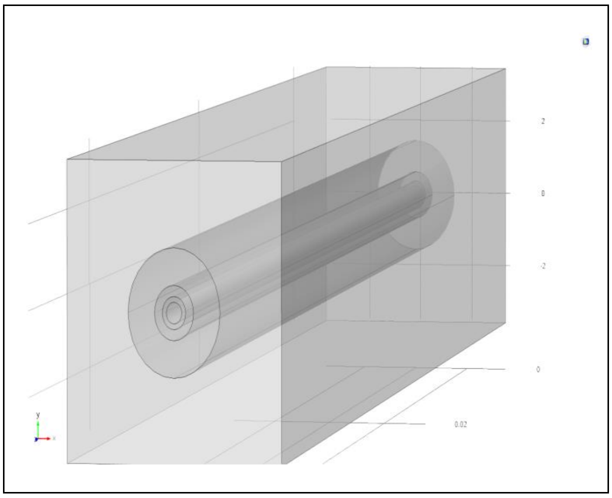

Fig. 3: 3D Geometry of Preconcentrator tube

Table 1. The material parameters of the pre-concentrator module (Wei Xoing, 2010)

S. No.	Materials	Dimensions: Internal Diameter (mm)	Dimensions: Outer Diameter (mm)	Density (Kg/m^3)	Heat Capacity at constant Pressure [J/(kg*K)]	Thermal conductivity [W/(m*K)]	Ratio of Specific Heats
1	Nichrome	0.5	-	8400	20	11.3	-
2	Air	-	-	1.225	1040	0.024	1.4
3	Borosilicate Glass	0.762	1.27	2230	750	1.44	-
4	Activated Carbon	-	-	600	0.34	0.17	-
5	Aluminum	3	-	2700	900	160	-
6	Teflon	3	-	2200	1400	0.23	-

The geometry of the model is then drafted along with the selection of element type (essentially the shape function) for meshing the structure. This is the most time consuming part of the work with much emphasis going towards proper element selection and input of appropriate material properties (www.comsol.com/patents). There are a handful of coupled field elements in COMSOL Multiphysics from which an appropriate one is selected and used for SAW analysis (Sharma *et al.* 1973). After the design of geometry, the problem domain is meshed according to the accuracy needs and available computer resources. If the structure is finely meshed, more accurate results are obtained but the memory and time requirements to solve the problem increases proportionately. So, often a balance is achieved between the two conflicting parameters namely, accuracy and size of the problem and the problem is finally solved optimally (Edmund *et al.* 2013). The optimized meshing for the simulation is determined by performing an independent grid study to minimize the modelling error. User defined free triangular elements was selected to mesh our specific 3-D model.

Table 2. Properties of mesh used in simulation

Number of degrees of freedom (DOF)	31766
No. of meshed points	4232
No. of elements	7420
No. of boundary elements	1042
No of vertex elements	56
Minimum element quality	0.623

The pre-concentrator device then simulated with different covering materials and studied by cyclic micro heating and cooling of the Nichrome heating element for the purpose of device temperature stability. A temperature profile for two materials (Teflon with Aluminum and Teflon without Aluminum) as covering material of pre-concentrator is studied.

3. ELECTRO-THERMAL ANALYSIS

For electro-thermal analysis, we are using the multiphysics capabilities of COMSOL to integrate the Joule Heating and heat transfer phenomena. The appropriate boundary conditions are utmost importance for achieving an accurate solution. The externally applied loads and excitation are supplied at this stage and it is an electrical voltage in the case of SAW devices (Venkatesan and Haresh M. Pandya, 2015). For instance in a static analysis, a watt is applied to the structure and its response is studied. The heating power (P) of a micro heater can be calculated by applying a voltage (V) across the two ends of a resister with a resistance (R). The power generated due to resistance can be calculated by Ohm's Law

$$P = V^2/R \qquad (1)$$

where, P is power in watts, V is the voltage across the resister, I is the current through the fibers, and R is the resistance.

A resistance of thin heating element can be found by the equation (2).

$$R = \rho L/wt \qquad (2)$$

where ρ is the resistivity of material, L is the length; w and t are the width and the thickness, respectively. By combining equation (1) and (2) we can obtain equation (3)

$$P=V^2wt/\rho L \qquad (3)$$

Therefore, by controlling the sizes of L, T and W of the heater, power of the heater can be controlled precisely. According to the above relations, a 5 watt power was applied to the heating element (Nichrome).

In this study, it is assumed that all electrical power generated is dissipated into heat. The entire Nichrome wire is assumed to be a heat source, and the heat dissipates into the device where resistive healing can occur. This problem can be solved for heat transfer analysis by the heat equation,

$$\rho C\frac{\partial T}{\partial t} + \nabla.(-k\nabla T) = Q \qquad (4)$$

where T is temperature, ρ is the density, C is the heat capacity (Cp, CV), k is the thermal conductivity, Q is a heat source or sink.

The multiphysics module from COMSOL 5.0 is used to solve the above equations. The initial temperature used during simulation is 20 °C. The Time dependent solver was used to determine the steady state temperature distribution of Preconcentrator tube. The simulation is carried out at a power input of 5 watt, which is applied to one end of heating electrode and other end is grounded. The inward heat flux is set at 5 Wm-2k-1 which incorporates for heat convection between Nichrome and air domain. Finally the model is simulated and output values for both Teflon alone and Teflon with Aluminium heat sink are computed and subsequently saved.

4. RESULTS & DISCUSSION

The simulated results are shown in fig. 4 and fig. 5. The results show that the final temperatures are affected primarily by the boundary conditions and the power input. Here we can see that at 5W power supply, the heater gives a temp rise of 420 °C with a uniform heat distribution with maximum temperature at the center of the heater that is NiCr wire. The following results show the cross-sectional view of a pre-concentrator tube wherein Teflon alone and Teflon with Aluminium heat sink are used as covering materials for temperature stability of that particular device. For both materials, computational results obtained are as given below.

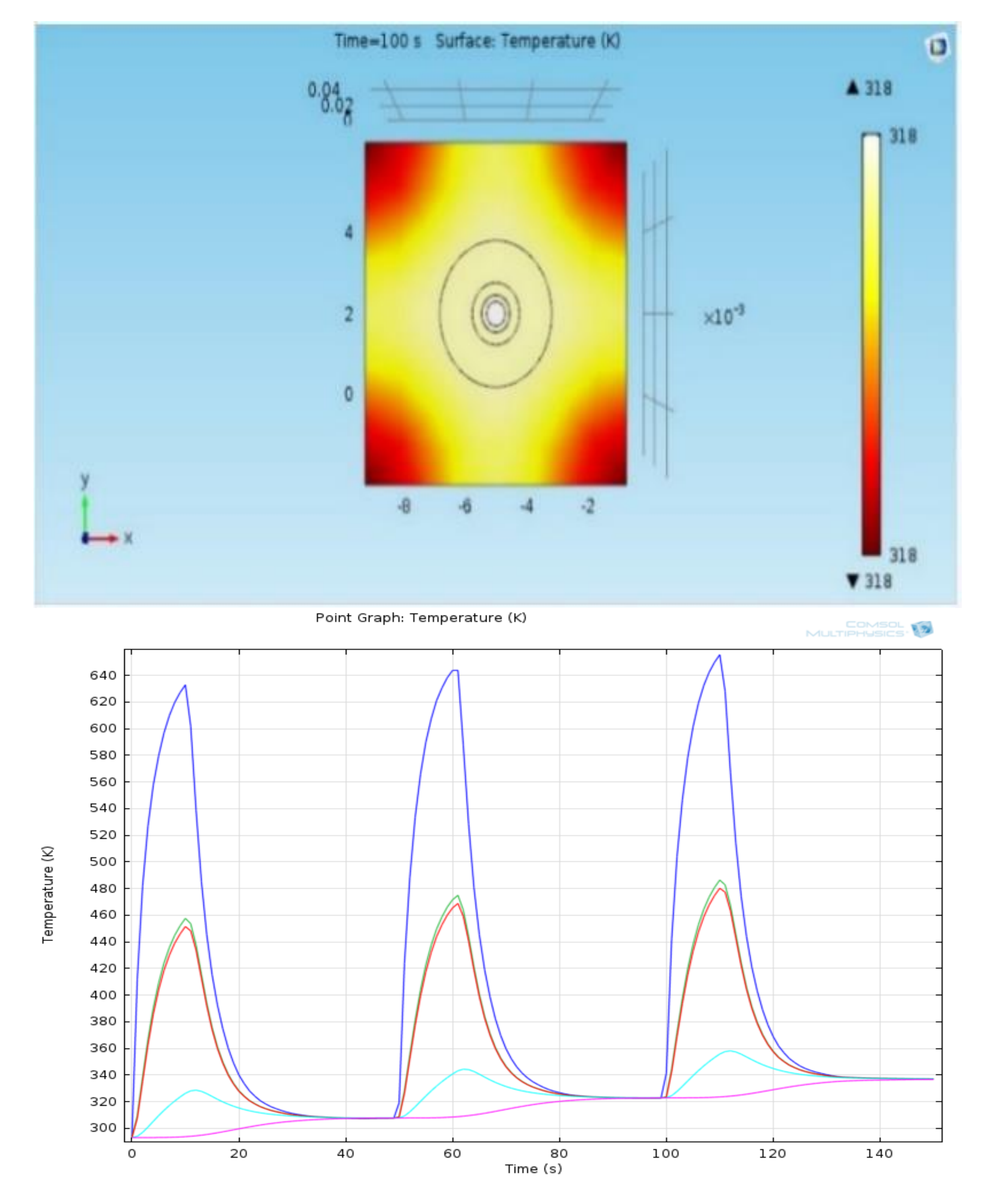

Fig. 4: Teflon without aluminum as a covering material - Heating and Cooling process - 3 Cycles: Surface plot and Time vs Temperature

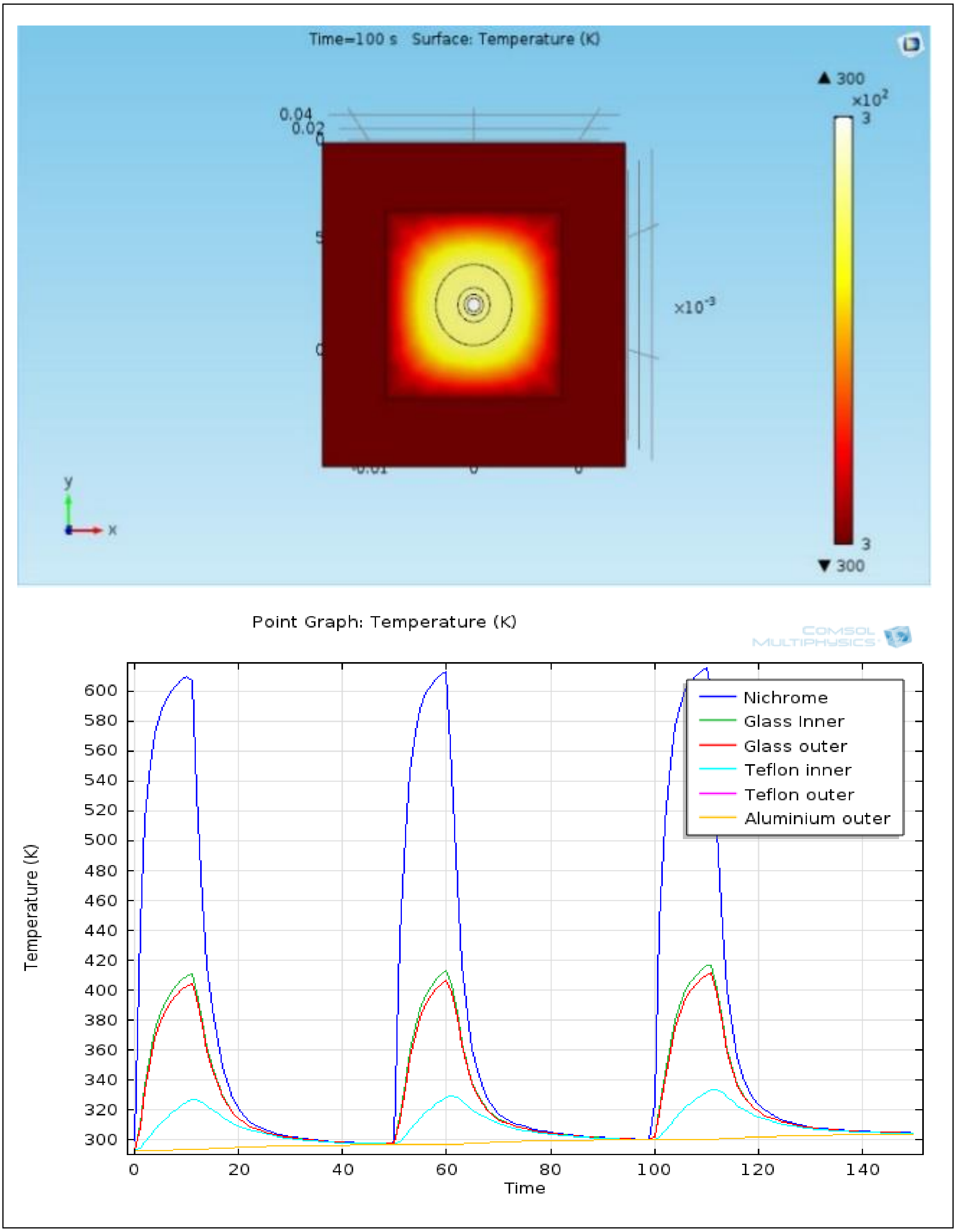

Fig. 5: Teflon with aluminum as a covering material - Heating and Cooling process - 3 Cycles: Surface plot and Time vs Temperature

It is observed from the simulation results that the temperature is higher in the center and goes on reducing towards the periphery. Further the temperature is found to be uniform over certain area of adsorbent region. However, the device have good temperature stability while using Aluminum with Teflon heat sink as a covering material. Whereas, while using Teflon without Aluminium heat sink, the device temperature was increased 10 kelvin per every cycle of successive heating and cooling.

4. CONCLUSION

From our present work, we conclude that it is better to maintain the temperature stability of pre-concentrator, by employing Teflon with Aluminium as a covering material. While using Teflon alone as a covering material, 5 K of device temperature is increased in every cycle and thus it can be conveniently avoided as a covering material. Thus this modelling and simulation study convincingly points to a better design and development of the pre-concentrator tube with Teflon and Aluminum in the future. Future study will also include the effect, behaviour and geometry of Nichrome wire in a helical shaped structure over a glass tube on the temperature profile studied for the design of better sensing GC based SAW Sensors.

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CONFLICTS OF INTEREST

The authors declare that there is no conflict of interest.

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