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Regular paper

Hollow Core-based Photonic Crystal Fiber Sensor : Design and Performance Development of Chemical Sensing in THz wave Propagation

Journal of Electrical Systems

This paper recommends a modified circular-shaped hollow-core photonic crystal fiber (H-PCF) based optical chemical sensor in the terahertz (THz) range (e.g., 1.0 THz ≤ f ≤ 3.0 THz). The developed structure is numerically assessed using the fully vectorial finite element technique (FV-FEM) and perfectly matched layer (PML) boundary conditions in the COMSOL Multiphysics software program. In this case, the fiber core is penetrated by chemical analytes. According to the results of the FV-FEM numerical analysis, the proposed optical H-PCF sensor exhibited very high relative sensitivities of 93.54%, 94.73%, and 92.50% for three chemicals at 1.6 terahertz (THz), namely, ethanol (n = 1.354), benzene (n = 1.366) and water (n = 1.330), respectively. Moreover, at 1.6 terahertz (THz), the low confinement losses are 4.89Ł10^{-7} dB/m, 1.66Ł10^{-7} dB/m, and 4.88Ł10^{-6} dB/m for three similar chemicals, and the corresponding effective areas are 9.41Ł10^{-8} m^2, 9.38Ł10^{-8} m^2, and 8.44Ł10^{-8} m^2, respectively. In addition, the effective material loss, effective mode index and total power fraction are also concisely explained here. Zeonex (Cyclo-Olefin Polymer) was selected as the fiber background material because it provides high sensing performance and low confinement loss throughout the terahertz (THz) regime. Because of its exceptional sensitive response and incredibly low confinement loss, this suggested sensor might be very useful for chemical identification. This proposed sensor can be fabricated using 3D printing method. Furthermore, we anticipate that our proposed sensor will be widely used in chemical and gas sensing, biomedicine, bio-sensing experiments, industrial regions, material investigations, nano-optics, healthcare, and other terahertz (THz) waveguide communication applications.

Keywords:Optical chemical sensor; Relative sensitivity; Confinement loss; Effective area, THz wave transmission.

1. Introduction

Chemicals, including ethanol, benzene, and water, are essential substances with significant importance in human life, industry and manufacturing, energy production, medicine and healthcare, food and agriculture, environmental protection, and scientific research. Their properties and uses highlight their significance in various aspects of human civilization and the natural world [1],[2]. Sensing chemicals anywhere atop the earth is a required endeavour, and identifying an unknown chemical is always a challenging and captivating issue for research. Ethanol is considered the major ingredient of chemicals and is widely utilized for numerous purposes. Most chemical solutions are composed of alcohol and water, which are regarded as the main analysers. Due to the colourlessness and lack of flow of alcohol, human health is at risk from a few of these toxins. Thus, a great deal of research into chemical analyte detection has been necessary. In order to fulfil people's

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requirements, researchers are developing and constructing extraordinary types of sensors [2]. For the safety of our health, there is a critical need for advanced sensing solutions capable of addressing these challenges and providing reliable and efficient chemical detection and analysis capabilities. Photonic crystal fibers (PCFs) have become increasingly popular in sensing and communications applications due to their numerous remarkable optical characteristics, particularly greater birefringence, decreased scattering loss, decreased effective material loss, greater sensitivity, and higher core power fraction, since its creation in 1996 [2],[3]. Novel opportunities for developing photonic instruments for sensing and communication applications have been made possible by photonic crystal fibers (PCFs). This particular kind of glass fiber design permits the application of a wider range of optical qualities, such as reduced loss, higher effective core area, enhanced transparency, and indefinite single-mode operation [1], [2], [3].On the other hand, PCF-based sensing equipment has been employed in a range of practical applications, including chemical and detecting of dangerous gases, diagnosing biological tissues, and finding cancer cells, respectively, because of its tiny size and excellent sensibility [1],[3],[4].The terahertz (THz) radiation band is a tiny band in the spectrum of electromagnetic energy (0.1 to 10 THz) that has recently attracted much attention because of its possible use. This spectrum of radiation is frequently employed since it is between the infrared and microwave zones, implying that it has no harmful impact on the environment or people [2], [3], [4]. PCFs are commonly classified into the following groups based on their core configuration: hollow-core, porous-core and solid-core. Of these three varieties, the first is unsuitable for chemical sensing; a hollow-core PCF is the most suitable selection since it offers the widest field for interaction between the radiation and the analyzer [3], [5], [6]. Moreover, a certain wavelength of light is injected into the PCF so that the tested analytes can propagate through the core. The refractive index of the waveguide affects the properties of lightpropagation; therefore, light of the same wavelength will move at different speeds depending on the analyte. It is possible to swiftly and precisely identify the properties of the tested analytes by receiving and evaluating the incoming signal[2],[6]. In recent years, scientists have proposed a huge number of PCF-based sensors that use THz signal propagation. Shuvo Sen et al. proposed H-PCF fiber arrangements around a hexagonal-shaped covering with a rotated hexa core. The structure of H-PCF has been clarified to achieve reduced confining loss and greater sensitivity in chemical-based detection. The sensor provides relative sensitivities of 81.46%, 82.26%, and 79.22% for three chemicals at 1 THz: ethanol, benzene, and water[1].This paper presents a study on designing a photonic crystal fiber (PCF) optimized for detecting hydrogen cyanide (HCN) gas, focusing on achieving high sensitivity and low confinement loss. The implementation of the suggested PCF is predicted using finite element method (FEM) simulations, which show circular air hole layers surrounding the core. At a wavelength of 1.533 µm, the results show a minimum confinement loss of 1.5 ×10-3 dB/m and a high relative sensitivity of 65.13%, indicating that it is suitable for industrial and medical applications requiring HCN detection [7].Kawsar Ahmed et al. suggested an extremely perceptive photonic crystal fiber (H-PCF) for chemical sensing, featuring a modified hexagonal structure optimized for increased chemical sensitivity. The PCF exhibited notable sensitivity to ethanol, water, and benzene, along with essential properties such as confinement loss and nonlinearity. The study highlighted its suitability for telecommunications, chemical sensing, and biosensing applications, showing a greater sensitivity response of 53.22%, 48.19%, and 55.56% for ethanol, water, and benzene detection at the regulating wavelength k = 1.33 μm [8].Rakib Hossen et al. discussed a novel photonic crystal fiber (PCF) design for detecting alcohols like ethanol, butanol, and propanol using terahertz (THz) spectrum sensing. By utilizing a hexahedron core and heptagonal cladding with circular air holes, the PCF demonstrates high sensitivity and low confinement losses at 1 THz, making it suitable for various applications, including in the food and beverage industry. This study highlights the potential of this PCF sensor for improving safety protocols by efficiently detecting alcohol in beverages [9].

In the present investigation, our proposed H-PCF sensor has a large circular air hole (CAH) in the core area and four-quarters circular-type air holes in the cladding region. The structure of H-PCF has been elucidated to reduce confinement loss and increase sensitivity in chemical sensing. Superior results in terms of relative sensitivity at 93.54%, 94.73%, and 92.50% are obtained with our suggested H-PCF sensor for three substances at 1.6 THz: ethanol (n=1.354), benzene (n=1.366), and water (n=1.330). Furthermore, it has low confinement losses of 4.89×10-7 dB/m, 1.66×10-7 dB/m, and 4.88×10-6 dB/m for three similar chemicals. Additionally, in comparison with earlier publications [1],[2],[6],[8] the recommended H-PCF structure here has very low confinement loss and high relative sensitivity (94.73%) for benzene at 1.6 THz.

2. Sensor Design and Theoretical Modelling

In the present investigation, circular air holes rather than elliptical holes have been used for the core region to reduce fabrication complexity. We provide a simple PCF optical chemical-sensor framework to improve the relative sensitivity while minimizing effective material loss and overcoming manufacturing challenges[10].Fig. 1. shows the sectional view and extension of the suggested sensor's core region, which includes the centre of a circular shape and the four-quarters circular-type clad portions [11].

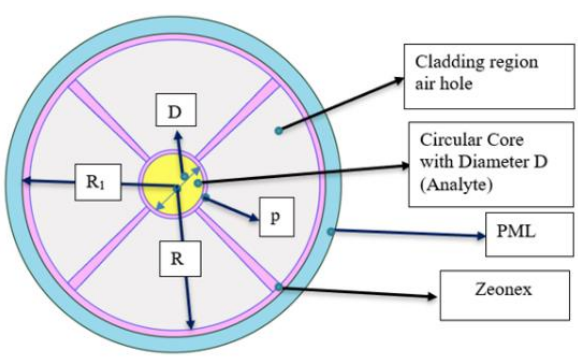


Fig. 1. Designed view of proposed hollow core-based PCF chemical detection sensor

A single, circular air hole is in the middle of the constructed structure of the suggested PCF. Four-quarters circular-type air hoes are put in a periodic configuration to produce the dielectric medium of the fibres in the cladding portion [11]. The distance between the two opposing edges of the core, represented by the letter D, is its diameter. The four-quarter circular type has a radius of R and a fiber radius of R_1, where R = 2.2811×D and R_1 = 2.471×D, and D=340 μm. These settings were established through trial and error since the suggested sensor had desired properties in specific situations. Along with the following cladding air holes, the symbol p, where p = 20 μm, denotes the distance between the nearest cladding arm and the core. There is a 4° angle difference in the spacing between the two nearby cladding air holes. Every design parameter is connected to a single factor, D, to simplify the production process. The outermost layer of the fiber, known as the PML, is 10% of the total size of the optical fiber [11]. In order to stop reflections back into the core, the PML's main function is to absorb light signals that leave the core and travel toward the cladding. Our proposed hollow-core PCF for the chemical detector employs Zeonex, the commercial name for Cyclo-Olefin Polymer (COP) [3], as the bulk material because of its minimal material absorbance loss, reliable reflecting indices across a large frequency range, and with the most stable index of refraction (n = 1.53) between 0.1 and 3 THz [5].HC-PCFs guide light through a hollow core surrounded by a photonic crystal cladding, often leveraging mechanisms like photonic bandgap guidance or anti-resonant effects. The segmentation of the computational region into circular areas within a finite number of dimensions is known as meshing. Fig. 2 illustrates these phenomena that were taken into account during the simulation. Elevating the mesh density can greatly enhance light transmission in the direction of the sensor, hence simplifying the numerical analysis and increasing the sensor accuracy. In this simulation, smaller element sizes and physics-controlled meshing are selected for meshing [12].

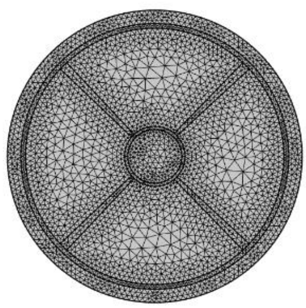
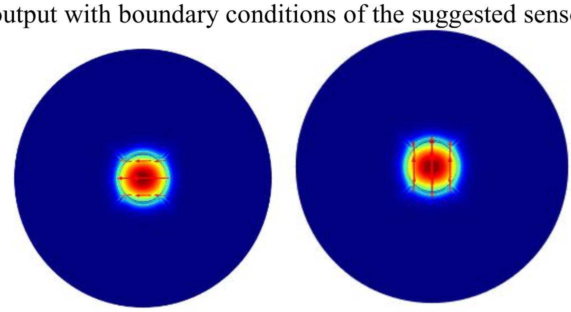
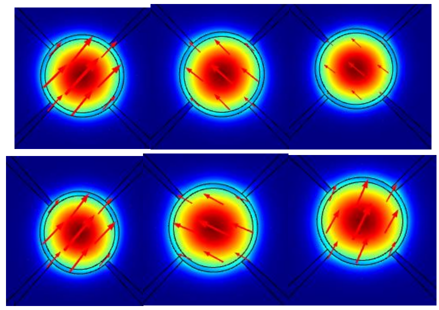


Fig. 2. Meshing output with boundary conditions of the suggested sensor.



(a) X Polarisation (b) Y Polarisation

Fig. 3. Light Confinement in the PCF-based chemical sensor's core



(a) X polarisation (b) Y polarisation

Fig. 4. Light mode distribution of H-PCF-based optical chemical sensor

Figs. 3(a) and 3(b) illustrates Light Confinement in the PCF-based chemical detection of the Proposed sensor 's core. Figs. 4(a) and 4(b) display the light mode variations of the PCF sensor at x-pol and y-pol at 1.6 THz, respectively, where the suggested sensor was filled with ethanol, benzene, and water, in that order. The x- and y-polarized sensitivities of the planned H-PCFs both increased due to the clear passing of the light confinement at the core. It is observed that distinct polarizations result in distinct light intensities being distributed across the fiber; consequently, there is a fascinating difference in the optical filaments' sensitivity, leakage loss, and other characteristics. However, in this arrangement, light in both polarizations passes through the core region to a logically equal degree [13]. The figures all demonstrated how tightly confined light is inside the core, which is necessary for excellent sensitivity.

3. Numerical Interpretation

To determine the fiber's general properties, numerical analysis is required. Different numerical approaches are advised for different PCF microstructures when it comes to electromagnetic analysis. [14]. To guarantee the correctness of the outcomes, the FV-FEM is employed in this instance throughout the whole numerical calculation. Here, COMSOL Multiphysics version 5.5 was utilized to investigate the suggested PCFs through the selection of a finer mesh analysis mode. The strength of the interaction between matter and radiation determines the delicate nature of the chemical adulteration sensor, as per the Beer-Lambert law. Equation (1) illustrates how this operation principle is applied to the recommended sensor, where evaluations are dependent on fluctuations in the proportion of absorption at a given frequency [5].

$$I(f) = L_0(f)e^{-r\alpha_m l_c} \tag{1}$$

Here, $I(f)$ indicates the electromagnetic radiation strength when the SUT is filled in the THz waveguide. (Sample Under Test), $L_0(f)$ is the intensity in the absence of the SUT, r represents the sensor's relative sensitiveness, and l_c is the waveguide's length relative sensitivity, which demonstrates the sensor's ability to detect changes in the SUT.

The following equation was used for estimating the effective area (EA). [4], [15].

$$A_{eff} = \frac{[\int I(rd)rddrd]^2}{[\int I^2(rd)drd]^2} \tag{2}$$

In this instance, A_{eff} is theeffective area, *I (r)* is the cross-sectional electric field intensity, and $[I(rd) = |E_t|^2$.

We realize that all power transmission occurs within the PCF framework. The total power fraction (PF) is obtained by using the equation that follows (1).

$$\eta = \frac{\int_i S_z dA}{\int_{all} S_z dA} \tag{3}$$

Here, the nominator integration represents the center or area covered in cladding, and η is the total power fraction. Furthermore, the entire cross-sectional area is determined using multiplying the denominator $S_z$by the pointing vector. [14] .

The following phrase may be used to simply quantify Confinement loss[9], [16].

$$L_c = 8.686 \times K_0 I_m[n_{eff}] \ (dB/m) \tag{4}$$

Here, $K_0 = \left(\frac{f}{c}\right)$, c id the photo speed and f is frequency. Additionally, the imaginary component $I_m(n_{eff})$ indicates the effective refractive index.

Relative sensitivity is the primary sensing agent that reveals the presence and concentration of any detecting analytes. For calculating the relative sensitivity (RS), we implement the following equation [17].

$$R = \frac{n_r}{n_{eff}} \times E \tag{5}$$

Here, n_r and n_{eff} correspondingly symbolize the refractive index (RI) and effective refractive index (ERI). Additionally, it is believed that the overall interaction between the material and the light is approximated as [5]

$$E = \frac{\int_{sample} R_e(E_x H_y - E_x H_y) dxdy}{\int_{total} R_e(E_x H_y - E_x H_y) \ dxdy} \times 100 \tag{6}$$

$H_x$and $H_y$imply for the magnetic fields of the x and y components. similarly,E_x and E_x represent the electric fields of the x and y components.

4. Simulation Outcomes and Discussions

The proposed H-PCF is assessed using FEM in conjunction with the sample under test (SUT). The refractive indices of the various chemical samples at room temperature are displayed in Table 1. An optical snooper, a spectral analyzer, an exhibit unit, and a terahertz light source are the fundamental components of this type of sensor apparatus. For the best precision, refreshing beverage mixing of the testing data and a laser source of light with a restricted bandwidth are needed. Any conventional technique will be used to insert the data into the core before turning on the light source. The analyzer will measure the power and calculate the effective refractive index of the light beam once it has entered the PCF and been picked up by the photodetector. Environmental variations, particularly temperature and humidity, can significantly affect the performance of photonic sensors. These effects arise from changes in the sensor's physical structure, optical properties, or surrounding medium, which influence its ability to accurately detect or measure signals.Therefore, the mathematical formulas required to ascertain the relative sensitivity of a proposed sensor and other guiding factors will be coded into a computer [5]. The simulated results were inserted into Origin Pro software and then the relative sensitivities curves as well as other results curves were obtained with respect to different frequencies in the terahertz range.

Table 1 Refractive indices of different chemical samples at room temperature.

Type of Chemical	Refractive Index
Ethanol	1.354
Benzene	1.366
Water	1.330

The diameter of the circular core, which is set to D =340 μm, is primarily considered to be a measure of the relative sensitivity of the detector. This research was conducted at a 1.6 THz frequency response. The relative sensitivity responses with frequency for both the x and y polarizations with ideal design specifications are displayed in Figs. 5 and 6. As the frequency increases, the relative sensitivity plots cover fewer dimensions, which leads to a gradual decrease in the frequency [17]. Furthermore, it has been noted that the low frequency range of 1 to 1.60 THz increase the relative sensitivity of ethanol, benzene, and water, which is then shown to decrease for the high spectrum of frequencies of 1.70 to 3 THz.

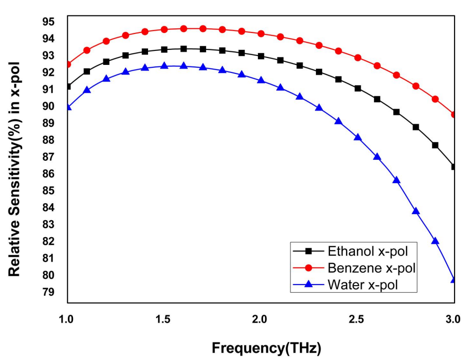


Fig. 5. The proposed H-PCH relative sensitivity (x-pol) to functional frequency for several chemical samples within the range of frequencies of 1.0 to 3.0 THz.

Furthermore, because benzene has a greater refractive index than the other two materials, the suggested sensor is more sensitive to benzene than the other two analytes. The greatest relative sensitivity for benzene, as shown in the accompanying figures, is 94.733% and 94.737% for the x and y polarization modes, respectively, which surpasses that of the cited works [1 − 5].

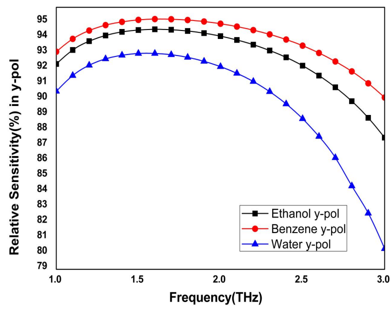


Fig. 6. The proposed H-PCH's relative sensitivity (y-pol) to functional frequency for several chemical samples within the range of frequencies of 1.0 to 3.0 THz.

Accordingly, Fig. 7 shows the EML design of the suggested sensor for various operating frequencies. The figures above show that the EML operates at 1.6 THz. At the optimal core diameter, which is a limited area, the EML varies for different chemical analytes at approximately 0.00819 cm^{-1}, 0.00763 cm^{-1}, and 0.00962 cm^{-1}. Nonetheless, analytes with a higher refractive index have a lower EML than those with a lower refractive index because they allow lighter particles to pass through them more easily under continuous operation circumstances. As shown in Fig. 8, the sensor displays similar features at different operating frequencies. Less light passes through the area of low-index cladding, allowing the solid substance between the cladding and core to absorb less light at higher frequencies. Higher frequencies have a lower loss, which makes sense [1].

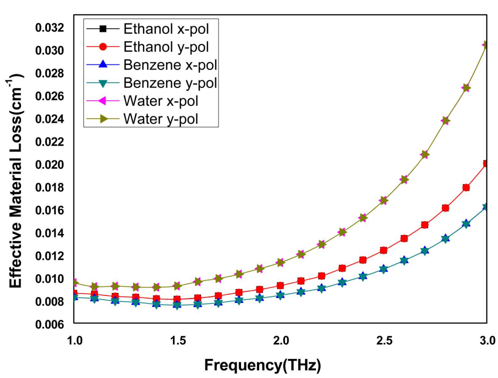


Fig. 7. For several chemical samples, the effective material loss is plotted against the functional frequency of the developed H-PCH within the range of frequencies of 1.0 to 3.0 THz.

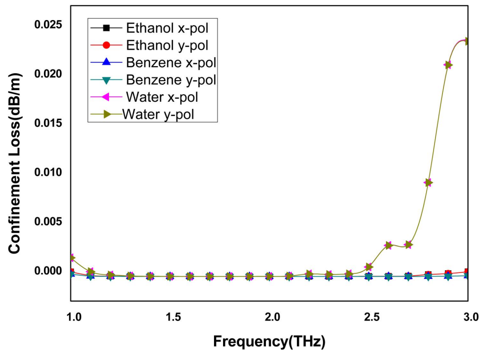


Fig. 8. Confinement loss for several chemical samples spanning the frequency range of 1.0 to 3.0 THz vs the functional frequency of the proposed H-PCH.

Fig. 8 displays the confinement loss feature vs frequency at appropriate settings. It can be seen that the confinement loss exhibits a comparable response within the frequency range of 2 to 3 THz, and it decreases as the frequency increases [18]. The confinement losses at 1.6 THz are 4.89×10^{-7} dB/m, 1.66×10^{-7}dB/m, and 4.88×10^{-6} dB/m for specific chemicals such as ethanol, benzene, and water constantly.

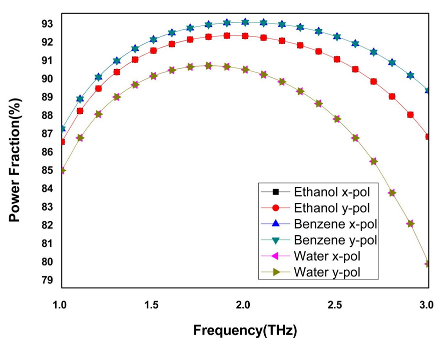


Fig. 9. Power ratio of the developed H-PCH vs. its useful frequency for several chemical samples at frequencies between 1.0 and 3.0 THz.

As previously stated, the two primary losses in PCF-based sensors are the EML and CL. Fig. 9 shows the total power fraction of the proposed sensor created. For different kinds of chemical samples, the CL given by the sensor under normal conditions are 4.89×10^{-7} dB/m, 1.66×10^{-7} dB/m, and 4.88×10^{-6} dB/m for ethanol, benzene and water, in that order. This is an improvement above the findings from previous research in Refs.[4], [7].

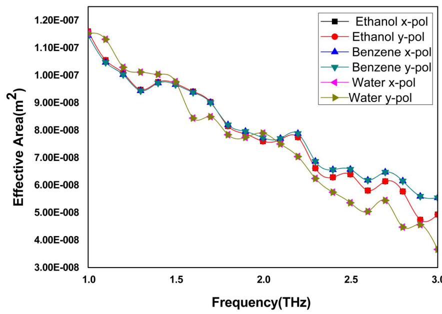


Fig. 10. For various chemical samples, the effective area vs the functional frequency of the suggested H-PCH throughout the frequency spectrum of 1.0 to 3.0 THz.

Fig. 10 displays the effective area versus frequency of the suggested H-PCF structure with ideal parameters. According to the frequency range of 1 to 3 THz, this visual outcome shows that the effective area decreases as the frequency increases [19], [20]. Furthermore, the greater effective area indicates that the terahertz (THz) wave pulse had low confinement loss and a higher relative sensitivity. Here, the effective areas of ethanol, benzene, and water are 9.41×10^{-8} m^2, 9.38×10^{-8} m^2, and 8.44×10^{-8} m^2, respectively, at a frequency of 1.6 THz.

Fig. 11 shows the effective mode index as a function of frequency for ideal parameters. It is clear that the effective mode index rises as the frequency increases. Here, 1.25 is used to introduce the effective mode index, and 1 THz is used to introduce the frequency. For the ethanol chemical sample, it is evident that the effective mode index may reach its maximum value of 1.37 when the frequency is increased to 3 THz.

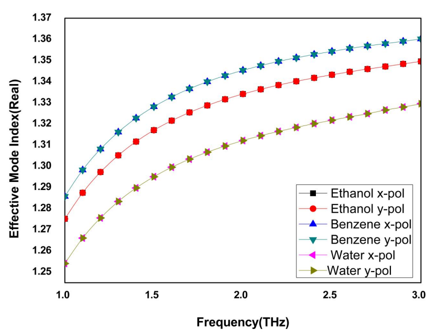


Fig. 11. Relation between frequensy vs effective refractive index (real) for various chemical samples throughout a frequency range of 1.0 to 3.0 THz.

A comparison table (Table 2) is computed for PCF-based sensing analysis. The following table indicates that the recommended sensor performs significantly superior to the liquid or chemical sensor described in relative sensitivity. A workable method for producing the proposed sensor is then examined. This hybrid sensor's sketch in the cross-section in Fig. 2 indicates that its core is circular. The fabrication challenge is decreased as all the holes in the core and cladding depend on only one constant (D) [25]. In the laboratory, several asymmetrically formed PCFs have been made using a range of construction methods. A close inspection of those fibers reveals that the produced PCFs are extremely similar to our modeled PCF.

Table 2 contrasting our suggested HC-PCF fiber with the previously mentioned PCF.

Reference	Finalizedfrequency(f)/wavelength(λ)	Sensing Sample	Relative Sensitivity	Confinement Loss (dB/m)
[1]	f =1 THz	Ethanol Benzene and Water	81.46%, 82.26% and 79.22%	5.85×10^{-08}, 6.07×10^{-08} and 5.84×10^{-08} dB/m
[6]	f =1.3 THz	Ethanol, Benzene, Water	78.8%, 77.8%, and 69.7%	2.19×10^{-10}
[16]	f =1.7 THz	Benzene, ethanol and water	89%, 88% and 86%	
[21]	f =1.0 THz	Ethanol, Benzene, water	78.56%, 79.76%, 77.51%	6.02×10^{-8} dB/m, 5.80×10^{-8} 8 dB/m, 5.74×10^{-8} dB/m
[22]	f =2.0 THz	camel and cowmilk	81.16% ,81.32 %	8.675×10^{-18}cm^{-1},.435 $\times 10^{-18}$cm^{-1}
[23]	f =1.0 THz	Ethanol	68.87%	-
[24]	f =1.7 THz	Benzene	89%	1.15×10^{-09} dB/m
This work 2024	**f =1.6 THz**	**Ethanol,Benzene, and Water**	**93.54%, 94.73%, 92.50%,**	**4.89×10^{-7} dB/m, 1.66×10^{-7}dB/m, 4.88×10^{-6} dB/m**

It is evident by comparing the structures of our suggested PCF with those of earlier published PCFs that the recommended fiber can be easily developed in the laboratory. The ideal fiber size for the suggested PCF is approximately 1.679 mm, indicating that the suggested sensor can be easily built in the laboratory

Fabrication feasibility: Photonic sensors, which rely on light-based mechanisms to detect various physical, chemical, or biological changes, offer high sensitivity and fast response times. However, their fabrication and practical application come with several challenges and limitations. But its geometric structure makes it possible to manufacture and employ in real-world situations. As a result, this might be a novel approach to chemical sample detection that is significantly more accurate, cost-effective, and has improved sensing capabilities compared to earlier studies.Until recently, a number of modern techniques for fabricating PCFs have been established (e.g., stack and draw approach, sol-gel, drilling, extrusion, 3D printing, etc.). To achieve this goal, we suggest using the stack and draw method or drilling or extrusion and 3D printing technologies to produce these specialized fibers since they enable the precise manufacture of all PCF types in a laboratory setting [2],[5].

Based on the table, our recommended chemical sensor could produce a lower EML. Furthermore, the sensitivity of this sensor has significantly improved, indicating that the present sensor version is suitable. Furthermore, the same method has recently been used to produce a Kagome-lattice fiber. It turned out to be rather accurate. These data indicate that the same process may be used to make our fiber. This is especially true given that our HC-PCF's architecture is far simpler than the Kagome type's[26].

5. Conclusion

Chemical components play a crucial role in various aspects of our lives, ranging from the natural world to industrial processes and healthcare. In this work, a fundamental structured PCF-based hollow core sensor for determining the identity of various chemical agents is proposed and thoroughly examined. The computer program COMSOL Multiphysics was utilized in the creation of this proposed H-PCF using the FEM process and the PML. The backdrop material for this suggested H-PCF sensor is Zeonex. The simulated findings of our experiment show that the relative sensitivities for ethanol, benzene and water are 93.54%, 94.73%, and 92.50%, correspondingly, at 1.6 THz frequency. Furthermore, the suggested H-PCF in the terahertz range yields confinement losses of 4.89×10^{-7} dB/m, 1.66×10^{-7} dB/m, and 4.88×10^{-6} dB/m for ethanol, benzene, and water, respectively. Additionally, the fibers exhibit very low effective material loss under optimal geometric circumstances at 0.00819 cm^{-1}, 0.00763 cm^{-1}, and 0.00962 cm^{-1}. Several domains, including food safety evaluation, biomedical and industrial fields, chemical sensing, business uses, medical technology, and other biological domains, will find it helpful.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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