Theoretical Considerations of Photonic Crystal Fiber with All Uniform-Sized Air Holes for Liquid Sensing

Abdul Mu’iz Maidi, Pg Emeroylariffion Abas, Pg Iskandar Petra, Shubi Kaijage, Nianyu Zou and Feroza Begum.

Abstract: A novel liquid-infiltrated photonic crystal fiber model applicable in liquid sensing for different test liquids—water, ethanol and benzene—has been proposed. One core hole and three air hole rings have been designed and a full vector finite element method has been used for numerical investigation to give the best results in terms of relative sensitivity, confinement loss, power fraction, dispersion, effective area, nonlinear coefficient, numerical aperture and V-Parameter. Specially, the assessed relative sensitivities of the proposed fiber with water, ethanol and benzene are 94.26%, 95.82% and 99.58%, respectively, and low confinement losses of $1.52 \times 10^{-11}$ dB/m with water, $1.21 \times 10^{-12}$ dB/m with ethanol and $6.01 \times 10^{-16}$ dB/m with benzene, at 1.0 µm operating wavelength. This novel PCF design is considered simple and can be easily fabricated for practical use, and the assessed waveguide properties has determined the potential applicability in real liquid sensing applications.

Keywords: photonic crystal fiber; liquid sensing; relative sensitivity; confinement loss

1. Introduction

Photonic crystal fiber (PCF) gained tremendous interest from researchers and manufacturers in the past few decades, after it was first introduced in the late 1990s [1]. This popularity arose due to its flexibility, in term of structural design, allowing air holes of different shapes and sizes to be embedded into the PCF, in order to manipulate different properties of the fiber. Refractive indices of the fibers can be uniquely changed to produce a desired effect, and correspond to certain optical properties [2]. This is in contrast to a conventional optical fiber, which is limited to altering refractive indices of the core and cladding only. A common photonic crystal fiber design is made up of pure silica glass, with air holes incorporated in the fiber axis. PCF generally has a high-index core within an air hole filled cladding, to give a hybrid of air-silica fiber with lower overall refractive index in its cladding than the refractive index in its core [3].

Some parameters that can be freely changed on a PCF are the design of its core and cladding, diameter of the integrated holes, number of air holes, and lattice pitch [4]. With these changes, remarkable results in optical properties are possible, such as high relative sensitivity, low confinement loss, high nonlinearity and single-modeness of the fiber. Consequently, the PCFs can potentially be applied in various optical applications, such as communication, as well as industrial and medical sensors [5–7]. An example of PCF utilization in such sectors are refractive index (RI) PCF sensors where recently an annular-core photonic crystal fiber (AC-PCF) was introduced to detect different concentrations
of glucose [8]. In addition, an octagonal PCF-based RI sensor has also been introduced to measure moisture content of transformer oil [9]. These significantly demonstrate the flexibility of PCF to be used for different sensor applications.

Many researchers have also suggested PCFs for other liquid sensing applications, such as in reference [10], where a liquid sensor for water, ethanol and benzene with a PCF design of three rings cladding and three elliptical holes in its core has been introduced. The simple PCF sensor exhibits confinement losses in the order of $10^{-7}$ dB/m, $10^{-8}$ dB/m and $10^{-11}$ dB/m with water, ethanol and benzene, respectively, and sensitivities of 62.60% with water, 65.34% with ethanol; and 74.50% with benzene, at 1.3 µm operating wavelength. Ahmed and Morshed [11] have proposed a PCF sensor design of 5 rings cladding and 9 holes in its core, using water, ethanol and benzene as test analytes. The liquid sensing PCF exhibits sensitivities of 45.05%, 46.87% and 47.35% with water, ethanol and benzene, respectively, at 1.33 µm operating wavelength. Additionally, at the same operating wavelength, confinement losses are about $10^{-15}$ dB/m with water and $10^{-14}$ dB/m with ethanol and benzene. A circular lattice PCF with 3 rings cladding and 16 holes in its core, has also been developed by Asaduzzaman et al. [12] for water, ethanol and benzene liquid sensing. At wavelength of 1.33 µm, the elaborate PCF sensor exhibits sensitivities of 48.85%, 49.14% and 49.29% with water, ethanol and benzene, respectively, and confinement losses in the range of $10^{-9}$ to $10^{-10}$ dB/m with all three liquid analytes. Another three rings liquid-infiltrated sensor has been proposed by Islam et.al [13] that exhibits acceptable values in sensitivities of 48.19% with water, 53.22% with ethanol and 55.60% with benzene. The design of the cladding air holes is of hexagonal arrangement and the PCF includes seven holes in its core; with the reported sensitivity values obtained at a wavelength of 1.33 µm. A different group of researchers [14] have proposed a PCF with 5 layers of cladding air holes and 9 holes in its cores, operating at 1.33 µm wavelength for sensing water, ethanol and benzene. The octagonal lattice sensor exhibits losses in the order of $10^{-13}$ dB/m with all three liquid analytes, and relative sensitivities of 52.07% with water, 56.75% with ethanol and 58.86% with benzene. A porous core PCF with 5 rings cladding has been presented by Sen et al. [15], with sensitivities of 57.0% with water, 57.18% with ethanol and 57.27% with benzene for liquid sensing application. The results are assessed at operating wavelength of 1.33 µm, with confinement losses in the order of $10^{-10}$ dB/m with water, and $10^{-11}$ dB/m with ethanol and benzene. Remarkably, another group of researchers [16] have demonstrated impressive results from their PCF design (with a hexagonal lattice of 5 layers cladding and a hexagonal-shaped core), which exhibits relative sensitivities of 88.93% with water, 91.87% with ethanol and 97.89% with benzene. Additionally, confinement losses of this sensor have been determined to be about $10^{-10}$ dB/m with all the three sensing liquids: water, ethanol and benzene. However, these admirable results are obtained, by having a great number of air holes along the fiber axis, which is a huge drawback during fabrication. On that note, references [10–16] have proposed photonic crystal fibers with large number of air holes in their axis and have incorporated intricate core designs, which consequently would make the PCFs difficult to manufacture and may lead to many errors during fabrication.

From the literature [10–16], it can be seen that good results, in terms of relative sensitivities and confinement losses, have been demonstrated from their PCFs, however, these have been obtained at the expense of intricate designs. In contrast, the proposed liquid sensor in this paper is a simple novel PCF, consisting of a uniform circular core holes and 36 air holes in its cladding, arranged in three rings of a hexagonal lattice structure. The design exhibits excellent results, with large power fraction, high relative sensitivity, low confinement loss, almost flattened chromatic dispersion, low effective area, high nonlinearity, and low numerical aperture. Relative sensitivities of the PCF with water, ethanol and benzene are 94.26%, 95.82% and 99.58%, respectively, and confinement losses are $1.52 \times 10^{-11}$ dB/m with water, $1.21 \times 10^{-12}$ dB/m with ethanol and $6.01 \times 10^{-16}$ dB/m with benzene, at wavelength of 1.0 µm. Furthermore, the PCF with all the three liquid analytes is able to operate as a single mode fiber.
2. Design

The proposed PCF sensor is a novel photonic crystal fiber design, in which the core of the structure is designed with one uniform circular air hole. Its core is placed on the cross-sectional center of the fiber, and the cladding constitutes the majority of the fiber structure, with multiple air holes positioned throughout the axis of the cladding region. A full vector finite element method (FEM) with perfectly matched layer (PML) has been implemented to simulate the proposed model. FEM is a numerical analysis method that has the capability of simulating and studying photonics structures. Figure 1 presents the proposed PCF model for liquid sensing application.

![Diagram of PCF model](image)

**Figure 1.** Design of the PCF-based sensor for liquid sensing.

Diameter of the air holes in the core and cladding is uniform, and is denoted as $d$. The core hole shall be infiltrated with liquid to serve the purpose of sensing the unknown analyte being inserted, with the cladding holes kept completely hollow. In the cladding, a total of 36 uniform-sized air holes is arranged in a hexagonal manner, with three rings. The distance between adjacent cladding air holes is known as the pitch, denoted as $p$. Perfectly matched layer (PML) is a boundary layer, which provides a conditional technique to evaluate propagation characteristics of leaky modes in PCFs. It aids in the absorption of leaked waveguide from the fiber and prevents light from being reflected back into the cladding and core.

The background material of the fiber has been selected to be pure silica. The corresponding air holes in the cladding are arranged with pitch distance $p = 1.8 \, \mu m$, with each cladding air holes and core holes having a diameter $d = 1.78 \, \mu m$. Moreover, the PML outside the fiber structure is elevated to be 10% of the cladding diameter to meet the boundary condition. Diameter of the total fiber: core, cladding and PML, is 14.4 $\mu m$.

3. Methodology

The proposed PCF is used for liquid sensing application, with various unknown liquid analytes to be injected into the core of the fiber for detection. Operating wavelength of the proposed PCF is between 0.6–2.0 $\mu m$. For this study, only three (3) different liquid analytes: water, ethanol and benzene, have been selected for testing the proposed PCF.
design for liquid detection. Figure 2 shows the refractive indices of the selected analytes at different operating wavelengths [17–20]. The refractive index of the core when injected with the analytes (i.e., refractive indices of water, ethanol and benzene) is higher than the cladding ($n \approx 1.00$), therefore, the guiding mechanism for this liquid-infiltrated PCF is through modified total internal reflection (m-TIR).

![Figure 2. Refractive index of liquid analytes: water, ethanol and benzene, at 0.6–2.0 µm operating wavelengths.](image)

The field distribution of the proposed PCF has been numerically analyzed using a full vector finite element method (FEM) in COMSOL Multiphysics software version 5.5. This simulation method divides the PCF geometry into small homogeneous triangular segments, known as meshing. The FEM process then utilizes Maxwell’s wave equation to solve these segments by accounting for neighboring subspaces. Overall, 58,833 mesh vertices, 111,868 triangular elements, 5,438 edge elements and 156 vertex elements have been used. The proposed PCF has an element area ratio of 0.007912, and total mesh area of 162.8 µm².

The optical properties that have been evaluated are effective refractive index, power fraction, relative sensitivity, confinement loss, chromatic dispersion, effective area, non-linear coefficient, numerical aperture and V-Parameter; these properties are assessed to determine the practicability of the proposed PCF.

With silica as background material and the core hole that has been injected with the test analytes, the effective refractive index $n_{\text{eff}}$ can be quantified and modelled using the Sellmeier’s equation given by [21]:

$$n_{\text{eff}}(\lambda) = \sqrt{1 + \frac{B_1 \lambda^2}{\lambda^2 - C_1} + \frac{B_2 \lambda^2}{\lambda^2 - C_2} + \frac{B_3 \lambda^2}{\lambda^2 - C_3}}$$

where $\lambda$ is the operating wavelength, and $B_{i=1,2,3}$ and $C_{i=1,2,3}$ are Sellmeier coefficients of the specific material.
Power fraction $P$ is a measure of the amount of power flowing through the PCF at a specific region, and it is defined as the ratio of power in a particular region to that of the total fiber, expressed as [22,23]:

$$P = \left(\frac{\text{sample}}{\text{total}}\right) \frac{\int \text{Re}(E_x H_y - E_y H_x) \, dx \, dy}{\int \text{Re}(E_x H_y - E_y H_x) \, dx \, dy} \times 100$$  \hspace{1cm} (2)

where $E_x$ and $E_y$ are the transverse electric fields of the guided mode, whilst $H_x$ and $H_y$ are the magnetic fields of the guided mode.

Relative sensitivity $S$ determines the efficiency of the PCF of its practicability which gives an insight on the interaction between light and test liquid analyte. It is defined as [22,23]:

$$S = \frac{n_r}{n_{\text{eff}}} \times P$$  \hspace{1cm} (3)

where $n_r$ is the refractive index of the sensed material.

The confined light in the PCF is characteristically leaky, leaking from the core to the cladding and this is referred to as confinement loss $L_c$. It measures the extent of loss of light from the core region of the fiber, and can be quantified by [24,25]:

$$L_c = \frac{40\pi}{\ln(10)} \frac{\lambda}{\lambda} \text{Im}[n_{\text{eff}}] \times 10^6$$  \hspace{1cm} (4)

where $\text{Im}[n_{\text{eff}}]$ is the imaginary part of effective mode index.

Chromatic dispersion $D$ is a measure of the light guiding capabilities of the fiber and the degradation of the mode in the fiber. It is defined as [25,26]:

$$D = -\frac{\lambda}{c} \frac{d^2}{d\lambda^2} \text{Re}[n_{\text{eff}}]$$  \hspace{1cm} (5)

where $c$ is the speed of light and $\text{Re}[n_{\text{eff}}]$ is the real part of effective refractive index.

Effective area $A_{\text{eff}}$ quantifies the cross-section area covered by the PCF in transverse dimensions, and is defined as [22,25,27]:

$$A_{\text{eff}} = \left(\frac{\int \int |E|^2 \, dx \, dy}{\int \int |E|^4 \, dx \, dy}\right)$$  \hspace{1cm} (6)

Nonlinear coefficient is a measure of the ability of the fiber to confine high intensity light, and is defined as [25,28]:

$$\gamma = \left(\frac{2\pi}{\lambda}\right) \left(\frac{n_2}{A_{\text{eff}}}\right)$$  \hspace{1cm} (7)

where $n_2$ is the nonlinear refractive index.

Numerical aperture $NA$ is a measure of the ability of the PCF to collect the incident light into the fiber, and is defined as [29,30]:

$$NA = \frac{1}{\sqrt{1 + \frac{\pi A_{\text{eff}} f^2}{c^2}}}$$  \hspace{1cm} (8)

where $f$ is the operating frequency.

$V$-Parameter $V_{\text{eff}}$ examines whether the PCF is single-mode or multimode fiber, and it is expressed as [31,32]:

$$V_{\text{eff}} = \frac{2\pi r f}{c} \sqrt{n_{\text{eff}}^2 - n_{\text{cl}}^2}$$  \hspace{1cm} (9)

where $r$ is the radius of the core, $n_{\text{eff}}$ is the effective refractive index of core and $n_{\text{cl}}$ is the effective refractive index of cladding.
4. Results and Discussion

Performance of the proposed PCF with water, ethanol and benzene has been analyzed by considering different optical parameters including power fraction, relative sensitivity, confinement loss, dispersion, effective area, nonlinear coefficient, numerical aperture and V-Parameter. The test analytes, with refractive indices given in references [17–20], are filled into the core region and the PCF is simulated for a range of operating wavelength between 0.6–2.0 µm. Figure 3 shows the mode profile of the PCF with different analytes at operating wavelength of 1.0 µm, which show the interaction of light with the liquid analytes present in the core region of the fiber. The figure demonstrates that light is closely confined within the core of the PCF.

**Figure 3.** Mode profile of the proposed PCF with (a) water, (b) ethanol and (c) benzene, at wavelength of 1.0 µm.

Effective refractive indices of the proposed PCF sensor with the sensing liquid analytes (water, ethanol and benzene) are illustrated in Figure 4. It demonstrates that effective refractive index decreases linearly with respect to an increase in wavelength. This is based on the phenomenon that electromagnetic signal with smaller wavelength consistently propagates through high refractive index region, whilst electromagnetic signal with longer wavelength has stronger capacity to overflow to the cladding region of the PCF. As compared to water and ethanol, the refractive index of benzene is slightly higher, hence, the effective refractive index of the proposed PCF with benzene is the highest, followed by ethanol and then, water.

**Figure 4.** Effective refractive index of the proposed PCF with liquid analytes: water, ethanol and benzene.
The relationship between power fraction of the proposed PCF with water, ethanol and benzene, and operating wavelength is shown in Figure 5. It can be seen that power fraction of the PCF with benzene decreases as wavelength increases. However, power fractions of the PCF with water and ethanol initially increase at lower operating wavelength of 0.6 to 0.7 µm, before decreasing. The optical power goes through the proposed core for the propagation mode, and the decreasing behavior is due to light leaking from the core volume to the surrounding cladding as wavelength increases. Power fractions of the proposed PCF with water, ethanol and benzene are taken at operating wavelength of 1.0 µm, henceforth, all optical properties are taken at that wavelength as well. At 1.0 µm, the power fractions of the PCF are 91.60% with water, 93.06% with ethanol and 96.69% with benzene.

![Power fraction of the PCF sensor for water, ethanol and benzene against wavelengths.](image)

Figure 6 shows the relationship between relative sensitivity and operating wavelength of the proposed PCF, with all the liquid analytes. It can be observed from the figure that benzene exhibits the highest relative sensitivity of nearly 100% for all operating wavelengths. On the other hand, water and ethanol also display high sensitivity, with relative sensitivity increasing from 0.6 to 1.0 µm and then, subsequently decreasing as wavelength further increases. Relative sensitivity is closely related to the refractive index of the test analytes. Therefore, the proposed PCF with benzene has the highest sensitivity as it has a higher refractive index and followed by ethanol and benzene. At wavelength of 1.0 µm, sensitivities of the proposed PCF with water, ethanol and benzene are 94.26%, 95.82%, 99.58%, respectively.

Confinement loss is a measure of loss of light leaking from the core to the outer region, and the behavior of confinement loss of the proposed PCF with water, ethanol and benzene in relation to operating wavelength, is shown in Figure 7. In theory, confinement loss generally increases with respect to wavelength, as more light tends to leak out of the core into the cladding as wavelength increases. This can be seen in the figure below. However, as benzene has a higher refractive index than water and ethanol, confinement loss of the proposed PCF with benzene is also much lower. The confinement losses of proposed PCF with water, ethanol and benzene are $1.52 \times 10^{-11}$ dB/m, $1.21 \times 10^{-12}$ dB/m and $6.01 \times 10^{-16}$ dB/m, respectively, at 1.0 µm.
Figure 5. Power fraction of the PCF sensor for water, ethanol and benzene against wavelengths.

Figure 6 shows the relationship between relative sensitivity and operating wavelength of the proposed PCF, with all the liquid analytes. It can be observed from the figure that benzene exhibits the highest relative sensitivity of nearly 100% for all operating wavelengths. On the other hand, water and ethanol also display high sensitivity, with relative sensitivity increasing from 0.6 to 1.0 $\mu$m and then, subsequently decreasing as wavelength further increases. Relative sensitivity is closely related to the refractive index of the test analytes. Therefore, the proposed PCF with benzene has the highest sensitivity as it has a higher refractive index and followed by ethanol and benzene. At wavelength of 1.0 $\mu$m, sensitivities of the proposed PCF with water, ethanol and benzene are 94.26%, 95.82%, 99.58%, respectively.

Figure 6. Relative sensitivity of the PCF sensor with water, ethanol and benzene, at different operating wavelengths.

Confinement loss is a measure of loss of light leaking from the core to the outer region, and the behavior of confinement loss of the proposed PCF with water, ethanol and benzene in relation to operating wavelength, is shown in Figure 7. In theory, confinement loss generally increases with respect to wavelength, as more light tends to leak out of the core into the cladding as wavelength increases. However, as benzene has a higher refractive index than water and ethanol, confinement loss of the proposed PCF with benzene is also much lower. The confinement losses of proposed PCF with water, ethanol and benzene are $1.52 \times 10^{-11}$ dB/m, $1.21 \times 10^{-12}$ dB/m and $6.01 \times 10^{-16}$ dB/m, respectively, at 1.0 $\mu$m.

Figure 7. Confinement loss of the PCF sensor with water, ethanol and benzene, for different operating wavelengths.

Figure 8 shows chromatic dispersion of the proposed PCF with water, ethanol and benzene, with respect to operating wavelength. It can be observed from graph that chromatic dispersion increases as wavelength increases from 0.6 to 0.8 $\mu$m, before it decreases as operating wavelength is further increased, with all the liquid analytes. Moreover, dispersions are almost similar with all the three analytes, and with confinement losses at very low value. The values of dispersion of the proposed PCF with water, ethanol and benzene are $-0.0086$ ps/nm.km, $-0.00832$ ps/nm.km and $-0.0099$ ps/nm.km, respectively, at wavelength of 1.0 $\mu$m.

Figure 8. Chromatic dispersion of the PCF sensor with water, ethanol and benzene, for different operating wavelengths.
Figure 7. Confinement loss of the PCF sensor with water, ethanol and benzene, for different operating wavelengths.

Figure 8. Chromatic dispersion of the PCF sensor with water, ethanol and benzene, for different operating wavelengths.

The relationship between effective area and wavelength of the proposed PCF with water, ethanol and benzene, is illustrated in Figure 9. Effective area of the proposed PCF with the selected liquid analytes increases almost linearly with an increase in operating wavelength, as seen in the figure. Water has the highest effective area, followed by ethanol, and then benzene. Essentially, effective area is the measure of how much cross-sectional area is covered by the PCF in the transverse dimension. This is deduced by the electric fields in the fiber, and this property increases as wavelength increases. At wavelength of 1.0 \( \mu m \), the effective areas of the proposed PCF are 2.230 \( \mu m^2 \) with water, 2.089 \( \mu m^2 \) with ethanol and 1.708 \( \mu m^2 \) with benzene.

Figure 9. Effective area of the PCF sensor with water, ethanol and benzene, for different operating wavelengths.

Figure 10 shows the relationship between nonlinear coefficient and operating wavelength of the proposed PCF sensor with the liquid analytes. It can be observed that nonlinear coefficient of the PCF with water, ethanol and benzene decreases non-linearly as wavelength increases. From Equation (7), it shows that nonlinearity is inversely proportional to effective area, which is evident when comparing Figures 9 and 10 as they show contrasting behavior to one another. Since refractive indices of water and ethanol have almost similar values, nonlinear coefficients of the proposed PCF with the two analytes are also almost similar. Benzene has a slightly higher nonlinear coefficient value. The nonlinear coefficients of the proposed PCF with water, ethanol and benzene are 84.55 W\(^{-1}\)km\(^{-1}\), 90.26 W\(^{-1}\)km\(^{-1}\) and 110.39 W\(^{-1}\)km\(^{-1}\), at 1.0 \( \mu m \), respectively.
Figure 10 shows the relationship between nonlinear coefficient and operating wavelength of the proposed PCF sensor with the liquid analytes. It can be observed that nonlinear coefficient of the PCF with water, ethanol and benzene decreases non-linearly as wavelength increases. From Equation (7), it shows that nonlinearity is inversely proportional to effective area, which is evident when comparing Figures 9 and 10 as they show contrasting behavior to one another. Since refractive indices of water and ethanol have almost similar values, nonlinear coefficients of the proposed PCF with the two analytes are also almost similar. Benzene has a slightly higher nonlinear coefficient value. The nonlinear coefficients of the proposed PCF with water, ethanol and benzene are 84.55 W\(^{-1}\)km\(^{-1}\), 90.26 W\(^{-1}\)km\(^{-1}\) and 110.39 W\(^{-1}\)km\(^{-1}\), at 1.0 µm, respectively.

![Figure 10. Nonlinear coefficient of the PCF sensor with water, ethanol and benzene, for different operating wavelengths.](image)

In this liquid sensing PCF, it is desirable to obtain a high numerical aperture, to deduce its efficiency for sensing application. This property is dependent on the effective refractive index, which is the refractive index difference between the core and the cladding. Figure 11 illustrates the relationship between numerical aperture of the proposed PCF with water, ethanol and benzene, and operating wavelength. It can be observed that numerical aperture with these liquid analytes increases as wavelength increases. At higher wavelength, numerical aperture is greater. Numerical apertures of the proposed PCF with water, ethanol and benzene are 0.3534, 0.3636 and 0.3963, respectively, at wavelength of 1.0 µm.

![Figure 11. Numerical aperture of the PCF sensor with water, ethanol and benzene, for different operating wavelengths.](image)

Figure 12 demonstrates the relationship between V-Parameter of the proposed PCF with all liquid analytes and operating wavelength. V-Parameter is the property that determines whether the proposed PCF is operating in either single-mode or multi-mode. It is desirable to operate in a single-mode operation, to deter from any multi-mode distortions. As seen from the figure, all liquid analytes: water, ethanol and benzene are operating well as a single-mode fiber as all values are below 2.405 [31]. V-parameter generally decreases as wavelength is increased. The V-parameters of the PCF at 1.0 µm are 1.806 with water, 1.747 with ethanol and 1.980 with benzene.
Moreover, to give allowance in fabrication, a tolerance analysis is performed by varying selected structural parameters: its pitch size and diameter of the holes and examine the effect of these variations on the optical properties: relative sensitivity and confinement loss. Analysis in the order of ±1% and ±2% has been applied on the parameters of the proposed PCF, is shown in Table 1. It can be seen that with a change of ±1% and ±2% on the global parameters, only slight changes of about ±0.05, ±0.05 and ±0.01 for the proposed PCF with water, ethanol and benzene, respectively, in terms of relative sensitivities and variations of about ±0.21 × 10^{-11}, ±0.51 × 10^{-12} and ±0.50 × 10^{-16} for the proposed PCF with water, ethanol and benzene, respectively, in terms of confinement losses, in comparison with all liquid analytes: water, ethanol and benzene, at operating wavelength. It can be observed that numerical aperture is greater. Numerical apertures of the proposed PCF with all liquid analytes increases as wavelength increases. At higher operating wavelengths, V-Parameter is the property that determines whether the proposed PCF is operating in either single-mode or multi-mode. It decreases as wavelength is increased. The V-parameters of the PCF at 1.0 μm. with water, 1.747 with ethanol and 1.980 with benzene. This proves that with a slight variation in fabrication, the optimum values can still be maintained.

Moreover, to give allowance in fabrication, a tolerance analysis is performed by varying selected structural parameters: its pitch size and diameter of the holes and examine the effect of these variations on the optical properties: relative sensitivity and confinement loss.
PCF with water, ethanol and benzene, respectively, in terms of confinement losses, in comparison to relative sensitivity and confinement loss obtained with the optimum global parameters. This proves that with a slight variation in fabrication, the optimum values can still be maintained.

Table 1. Comparison among the variation in global parameters on optimum parameters at $\lambda = 1.0 \mu m$.

| Change in Global Parameters | Water Relative Sensitivity (%) | Ethanol Relative Sensitivity (%) | Benzene Relative Sensitivity (%) | Water Confinement Loss (dB/m) | Ethanol Confinement Loss (dB/m) | Benzene Confinement Loss (dB/m) |
|-----------------------------|--------------------------------|---------------------------------|---------------------------------|------------------------------|---------------------------------|-------------------------------|
| +2%                         | 94.29                          | 95.86                           | 99.59                           | $1.73 \times 10^{-11}$       | $1.41 \times 10^{-12}$         | $5.82 \times 10^{-16}$        |
| +1%                         | 94.27                          | 95.84                           | 99.58                           | $1.61 \times 10^{-11}$       | $1.35 \times 10^{-12}$         | $5.95 \times 10^{-16}$        |
| Optimum                     | 94.26                          | 95.82                           | 99.58                           | $1.52 \times 10^{-11}$       | $1.21 \times 10^{-12}$         | $6.01 \times 10^{-16}$        |
| −1%                         | 94.23                          | 95.80                           | 99.57                           | $1.41 \times 10^{-11}$       | $1.11 \times 10^{-12}$         | $6.39 \times 10^{-16}$        |
| −2%                         | 94.21                          | 95.77                           | 99.57                           | $1.32 \times 10^{-11}$       | $1.04 \times 10^{-12}$         | $6.51 \times 10^{-16}$        |

Lastly, a comparison between the proposed fiber and prior liquid infiltrated PCF is presented in Table 2. It can be observed from the table that the proposed PCF demonstrates the highest relative sensitivity and confinement loss, with all the liquid analytes. In comparison to the PCFs in references [10–16], it can be seen that the proposed PCF produces the best results: highest sensitivity, lower confinement loss, smaller dispersion, high nonlinearity and higher numerical aperture.

Table 2. Comparison of structure and performance among prior PCFs and proposed PCF at $\lambda = 1.0 \mu m$.

| No. of Rings | Structure | Relative Sensitivity (%) | Confinement Loss (dB/m) | Dispersion (ps/nm·km) | Nonlinear Coefficient ($W^{-1}km^{-1}$) | Numerical Aperture |
|--------------|-----------|--------------------------|-------------------------|-----------------------|----------------------------------------|-------------------|
| Core         | Cladding  |                          |                         |                       |                                        |                   |
| Ref. [10]    | 3         | 3 core holes             | 59.9 (W)                | $~10^{-7}$ (W)        | $-0.0104$ (W)                          | 99 (W)            |
|              |           | Circular holes in hexagonal | 62.7 (E)          | $~10^{-8}$ (E)        | $-0.0101$ (E)                          | 109 (E)           |
|              |           |                          | 78.8 (B)                | $~10^{-11}$ (B)       | $-0.0115$ (B)                          | 138 (B)           |
| Ref. [11]    | 5         | 9 core holes             | 43.3 (W)                | $~10^{-13}$ (W)       | -                                      | -                 |
|              |           | Circular holes in hexagonal | 44.31 (E)         | $~10^{-14}$ (E)       | -                                      | -                 |
|              |           |                          | 47.2 (B)                | $~10^{-15}$ (B)       | -                                      | -                 |
| Ref. [12]    | 5         | 16 core holes            | 46.3 (W)                | $~10^{-9}$ (W)        | -                                      | -                 |
|              |           | Circular holes in circle  | 46.5 (E)                | $~10^{-9}$ (E)        | -                                      | -                 |
|              |           |                          | 46.9 (B)                | $~10^{-10}$ (B)       | -                                      | -                 |
| Ref. [13]    | 3         | 7 core holes             | 51.6 (E)                | -                     | -                                      | -                 |
|              |           | Circular holes in hexagonal | 54.2 (B)          | -                     | -                                      | -                 |
| Ref. [14]    | 5         | 9 core holes             | 44.2 (W)                | $~10^{-13}$ (W)       | 4.2 (W)                                |
|              |           | Circular holes in octagonal | 47.3 (E)          | $~10^{-13}$ (E)       | 4.4 (E)                                |
|              |           |                          | 52.5 (B)                | $~10^{-13}$ (B)       | 4.9 (B)                                |
| Ref. [15]    | 5         | Porous core              | 57.3 (W)                | $~10^{-8}$ (W)        | 9.80 (W)                               |
|              |           | Circular holes in hexagonal | 57.9 (E)          | $~10^{-9}$ (E)        | 10.4 (E)                               |
|              |           |                          | 57.9 (B)                | $~10^{-9}$ (B)        | 11.9 (B)                               |
| Ref. [16]    | 5         | 1 core hole              | 91.2 (W)                | $~10^{-11}$ (W)       | 53.1 (W)                               |
|              |           | Circular holes in circle  | 94.0 (E)                | $~10^{-13}$ (E)       | 52.5 (E)                               |
|              |           |                          | 97.5 (B)                | $~10^{-10}$ (B)       | 58.9 (B)                               |
| Proposed PCF | 3         | 1 core hole              | 94.26 (W)               | $~10^{-11}$ (W)       | 84.55 (W)                              |
|              |           | Circular holes in hexagonal | 95.82 (E)       | $~10^{-12}$ (E)       | 90.26 (E)                              |
|              |           |                          | 99.58 (B)               | $~10^{-16}$ (B)       | 110.39 (B)                             |

Where W refers to water, E refers to ethanol and B refers to benzene.

In this sensing application, the hollow core hole needs to be injected with the liquid analytes. The infiltration of liquid into the core of the PCF can be accomplished through selective air hole filling technique [33], which has been experimentally studied by researchers with much success. The technique is capable of injecting liquids into the micro-structured core and cladding holes in the PCF. Other methods for injecting liquid analytes, that
have been proposed by various researchers include using multi-step injection-cure-cleave process [34], fusion splicer [35], and lateral filling [36].

5. Conclusions

A novel PCF based sensor with one liquid-infiltrated core hole and 36 cladding air holes arranged in a hexagonal lattice of three layers, has been proposed for liquid sensing application, with water, ethanol and benzene used as test analytes. A full vector FEM has been utilized for numerical analysis of the proposed PCF and assessment on waveguide properties in terms of power fraction, relative sensitivity, confinement loss, chromatic dispersion, effective area, nonlinear coefficient, numerical aperture and V-Parameter have been performed. The optimal results are obtained at 1.0 µm and depicts high sensitivities of 94.26% with water, 95.82% with ethanol and 99.58% with benzene, and high confinement losses of $1.52 \times 10^{-11}$ dB/m, $1.21 \times 10^{-12}$ dB/m and $6.01 \times 10^{-16}$ dB/m with water, ethanol and benzene, respectively. Furthermore, the proposed sensor operates as a single mode fiber with the three analytes. Ultimately, the results obtained above exemplify that the proposed fiber has the capability to be applied in optical communication and sensing applications in industrial and medical sectors, as used in this paper.

Author Contributions: Conceptualization, A.M.M. and F.B.; methodology, A.M.M. and F.B.; software, A.M.M., S.K. and F.B.; validation, P.E.A. and F.B.; formal analysis, A.M.M. and F.B.; investigation, A.M.M. and F.B.; resources, P.I.P. and F.B.; data curation, A.M.M. and F.B.; writing—original draft preparation, A.M.M.; writing—review and editing, P.E.A. and F.B.; visualization, P.E.A., N.Z. and F.B.; supervision, F.B.; project administration, F.B.; funding acquisition, F.B. All authors have read and agreed to the published version of the manuscript.

Funding: This research is funded by UNIVERSITI BRUNEI DARUSSALAM, grant number, UBD/RSCH/1.3/FICBF(b)/2019/008.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Not applicable.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Knight, J.C.; Birks, T.A.; Russell, P.S.J.; Atkin, D.M. All-silica single-mode optical fiber with photonic crystal cladding: Errata. Opt. Lett. 1997, 22, 484. [CrossRef]
2. Cordeiro, C.M.B.; Franco, M.A.R.; Chesini, G.; Barretto, E.C.S.; Lwin, R.; Brito Cruz, C.H.; Large, M.C.J. Microstructured-core optical fibre for evanescent sensing applications. Opt. Express 2006, 14, 13056. [CrossRef] [PubMed]
3. Leon, M.J.B.M.; Kabir, M.A. Design of a liquid sensing photonic crystal fiber with high sensitivity, birefringence & low confinement loss. Sens. Bio-Sens. Res. 2020, 28, 100335. [CrossRef]
4. Buczynski, R. Photonic crystal fibers. Acta Phys. Pol. A 2004, 106, 141–167. [CrossRef]
5. Lucki, M. Photonic Crystal Fibers with Optimized Dispersion for Telecommunication Systems. Recent Prog. Opt. Fiber Res. 2012. [CrossRef]
6. Kumar, S.; Bisht, A.; Bisht, A.; Singh, G.; Amphanwak, A. Design of photonics crystal fiber sensors for bio-medical applications. Opt. Meas. Syst. Ind. Insp. IX 2015, 9525, 95252B. [CrossRef]
7. Pinto, A.M.R.; Lopez-Amo, M. Photonic crystal fibers for sensing applications. J. Sens. 2012, 2012. [CrossRef]
8. Sharma, M.; Mishra, S.K.; Ung, B. Ultra-sensitive and large dynamic range refractive index sensor utilizing annular core photonic crystal fiber. SPIE 2019, 5, 1112305. [CrossRef]
9. Paul, A.K. Design and analysis of photonic crystal fiber plasmonic refractive Index sensor for condition monitoring of transformer oil. OSA Contin. 2020, 3, 2253. [CrossRef]
10. Maiti, A.M.; Yokasai, I.; Abas, P.E.; Nauman, M.M.; Apong, R.A.; Kajage, S.; Begum, F. Design and Simulation of Photonic Crystal Fiber for Liquid Sensing. Photonics 2021, 8, 16. [CrossRef]
11. Ahmed, K.; Morshed, M. Design and numerical analysis of microstructured-core octagonal photonic crystal fiber for sensing applications. Sens. Bio-Sens. Res. 2016, 7, 1–6. [CrossRef]
12. Asaduzzaman, S.; Ahmed, K.; Bhuiyan, T.; Farah, T. Hybrid photonic crystal fiber in chemical sensing. Springerplus 2016, 5. [CrossRef]
13. Islam, M.S.; Paul, B.K.; Ahmed, K.; Asaduzzaman, S.; Islam, M.I.; Chowdhury, S.; Sen, S.; Bahar, A.N. Liquid-infiltrated photonic crystal fiber for sensing purpose: Design and analysis. *Alex. Eng. J.* 2018, 57, 1459–1466. [CrossRef]

14. Ahmed, K.; Morshed, M.; Asaduzzaman, S.; Arif, M.F.H. Optimization and enhancement of liquid analyte sensing performance based on square-cored octagonal photonic crystal fiber. *Optik* 2017, 131, 687–696. [CrossRef]

15. Sen, S.; Chowdhury, S.; Ahmed, K.; Asaduzzaman, S. Design of a porous cored hexagonal photonic crystal fiber based optical sensor with high relative sensitivity for lower operating wavelength. *Photonic Sens.* 2017, 7, 55–65. [CrossRef]

16. Eid, M.M.A.; Habib, M.A.; Anower, M.S.; Rashed, A.N.Z. Highly sensitive nonlinear photonic crystal fiber based sensor for chemical sensing applications. *Microsyst. Technol.* 2020. [CrossRef]

17. Arif, M.F.H.; Asaduzzaman, S.; Ahmed, K.; Morshed, M. High sensitive PCF based chemical sensor for ethanol detection. In Proceedings of the 5th International Conference on Informatics, Electronics & Vision (ICIEV), Dhaka, Bangladesh, 13–14 May 2016; pp. 6–9. [CrossRef]

18. Malitson, I.H. Interspecimen Comparison of the Refractive Index of Fused Silica. *J. Opt. Soc. Am.* 1965, 55, 1205. [CrossRef]

19. Hale, G.M.; Querry, M.R. Bladder cancers respond to EGFR inhibitors. *Cancer Discov.* 2014, 4, 980–981. [CrossRef]

20. Moutzouris, K.; Papamichael, M.; Betsis, S.C.; Stavrakas, I.; Hloupis, G.; Triantis, D. Refractive, dispersive and thermo-optic properties of twelve organic solvents in the visible and near-infrared. *Appl. Phys. B Lasers Opt.* 2014, 116, 617–622. [CrossRef]

21. Akowuah, E.K.; Gorman, T.; Ademgil, H.; Haxha, S.; Robinson, G.K.; Oliver, J.V. Numerical analysis of a photonic crystal fiber for biosensing applications. *IEEE J. Quantum Electron.* 2012, 48, 1403–1410. [CrossRef]

22. Yakasai, I.K.; Abas, P.E.; Ali, S.; Begum, F. Modelling and simulation of a porous core photonic crystal fibre for terahertz wave propagation. *Opt. Quantum Electron.* 2019, 51. [CrossRef]

23. Yakasai, I.; Abas, P.E.; Kaijage, S.F.; Caesarendra, W.; Begum, F. Proposal for a quad-elliptical photonic crystal fiber for terahertz wave guidance and sensing chemical warfare liquids. *Photonics* 2019, 6, 78. [CrossRef]

24. Begum, F.; Namihira, Y.; Kinjo, T.; Kaijage, S. Supercontinuum generation in photonic crystal fibres at 1.06, 1.31, and 1.55 m wavelengths. *Electron. Lett.* 2010, 46, 1518–1520. [CrossRef]

25. Arif, M.F.H.; Hussain, M.M.; Islam, N.; Khaled, S.M.A. A nonlinear photonic crystal fiber for liquid sensing application with high birefringence and low confinement loss. *Sens. Bio-Sens. Res.* 2019, 22, 100252. [CrossRef]

26. Begum, F.; Namihira, Y.; Razzak, S.M.A.; Kaijage, S.F.; Hai, N.H.; Miyagi, K.; Higa, H.; Zou, N. Flattened chromatic dispersion in square photonic crystal fibers with low confinement losses. *Opt. Rev.* 2009, 16, 54–58. [CrossRef]

27. Hossain, M.; Podder, E.; Adhikary, A.; Al-Mamun, A. Optimized Hexagonal Photonic Crystal Fibre Sensor for Glucose Sensing. *Adv. Res.* 2018, 13, 1–7. [CrossRef]

28. Islam, M.S.; Sultana, J.; Ahmed, K.; Islam, M.R.; Dinovitser, A.; Ng, B.W.-H.; Abbott, D. A Novel Approach for Spectroscopic Chemical Identification Using Photonic Crystal Fiber in the Terahertz Range. *IEEE Sens. J.* 2018, 18, 575–582. [CrossRef]

29. Chowdhury, S.; Sen, S.; Ahmed, K.; Asaduzzaman, S. Design of highly sensible porous shaped photonic crystal fiber with strong confinement field for optical sensing. *Optik* 2017, 142, 541–549. [CrossRef]

30. Habib, A.; Anower, S.; Haque, I. Highly sensitive hollow core spiral fiber for chemical spectroscopic applications. *Sens. Int.* 2020, 1, 100011. [CrossRef]

31. Rana, S.; Saiful Islam, M.; Faisal, M.; Roy, K.C.; Islam, R.; Kaijage, S.F. Single-mode porous fiber for low-loss polarization maintaining terahertz transmission. *Opt. Eng.* 2016, 55, 076114. [CrossRef]

32. Yu, C.-P.; Liou, J. Selectively liquid-filled photonic crystal fibers for optical devices. *Opt. Express* 2009, 17, 8729. [CrossRef] [PubMed]

33. Huang, Y.; Xu, Y.; Yariv, A. Fabrication of functional microstructured optical fibers through a selective-filling technique. *Appl. Phys. Lett.* 2004, 85, 5182–5184. [CrossRef]

34. Xiao, L.; Jin, W.; Demokan, M.S.; Ho, H.L.; Hoo, Y.L.; Zhao, C. Fabrication of selective injection microstructured optical fibers with a conventional fusion splicer. *Opt. Express* 2005, 13, 9014. [CrossRef] [PubMed]

35. Cordeiro, C.M.B.; dos Santos, E.M.; Brito Cruz, C.H.; de Mato, C.J.; Ferreira, D.S. Lateral access to the holes of photonic crystal fibers—Selective filling and sensing applications. *Opt. Express* 2006, 14, 8403. [CrossRef] [PubMed]