Optimizations of optical polymer waveguide dimensions for ammonia sensor applications

Y M R Faozan¹, D Mahmudin¹, P Daud¹, Y N Wijayanto¹, G Sugandi¹ and A B Pantjawati²,*

¹Research Center for Electronics and Telecommunications, Lembaga Ilmu Pengetahuan Indonesia (P2ET-LIPI), Bandung, Indonesia.
²Department of Electrical Engineering Education, Universitas Pendidikan Indonesia (UPI), 40154, Bandung, West Java, Indonesia

*E-mail: usq.upi@gmail.com

Abstract. In this paper, we investigated the optimum dimension of waveguide for ammonia sensor applications. The waveguide material was poly methyl methacrylate (PMMA) on with glass substrate. The study was conducted by comparing the change in refractive index of analyte against electric field for each dimensions of waveguide. We simulated the variation of width and height by using the finite element method technique (FEM) in COMSOL Multiphysics®. The result shows the change of electric field depends on height of waveguide. The electric field change becomes the basic for sensor applications.

1. Introduction
Ammonia is a chemical compound with the formula NH₃. Ammonia is alkaline gas that is not colour, lighter than air, and has a distinctive aroma. Ammonia has a significant contribution to the presence of nutrients in the Earth, ammonia is caustic and can damage health living beings especially fish. Ammonia is the primary nitrogenous waste product of fish and also originates from the decay of complex nitrogenous/protein compounds [1, 2]. Toxicities in fish are most commonly due to abnormalities in water quality; poor water quality is one of the most common causes of morbidity and mortality in fish. Therefore, a complete water quality evaluation should be performed in every case. Acute exposure to poor water quality can result in sudden and significant mortality. Chronic exposure to suboptimal water quality conditions can cause immunosuppression and predispose fish to a variety of infectious diseases that ultimately lead to mortality.

Ammonia is present in two forms: ionized (NH₄⁺) and non-ionized (also called unionized, NH). Non-ionized ammonia is the most toxic form. The portion of total environmental ammonia that is present in the non-ionized form is dependent on pH and, to a lesser degree, on water temperature and salinity. Ammonia is more toxic in warmer water, at higher pH, and at lower salinity [1–3]. The higher the pH, the more ammonia is present in the non-ionized form; therefore, ammonia toxicity is worsened in aquaria that have higher pH. For every 1-unit decrease in pH, there is a tenfold decrease in non-ionized ammonia [2].

Optical sensors are recently being considered for many applications such as chemical sensors, biological sensors, and pressure sensors. Optical sensors have the advantage of detecting ammonia in water. Compared to electrical sensors, optical sensors have several advantages such as higher sensitivity by using optical interference, immunity to electromagnetic interference, and longer
lifetimes without the need for electrical contacts [1, 2]. Therefore, many of chemical sensors used optical sensors waveguides. The basic operation principle of optical chemical sensor is that when an optical sensor is exposed to a chemical, the signal traveling through an optical waveguide changes. Optimization of optical waveguides depends on dimension of waveguides [3, 4].

In this paper, we investigate the dimensions of waveguide optical sensors. The structure of waveguide in this study was channel waveguide. The channel waveguide has the same of width and height. The channel waveguides are extensively used, for example, within various laser diodes. The channel waveguide is small and has a single-mode channel waveguide with transverse dimensions, for example 1 µm. The single mode waveguide has high electric field. The dimension changes of waveguide influence the electric field. Thus, the electric field of the waveguide can change the power [5]. The change of power is basic principle for optical sensor.

The purpose of this study was to obtain the optimum dimensions of the channel waveguide for ammonia sensor application through simulation. We also evaluated some dimensions of waveguide (waveguide width and waveguide height) to get high value electric field and the linear change of electric field due to refractive index analyte. The simulation of channel waveguide gave the optimum height and width of waveguide. The result of simulation presented that the variety of dimensions influence on the electric field linearly.

2. Experimental Methods
We used of the commercial FEM software to simulate the channel waveguide. Many commercial software is based on FEM such as Analysis3D, FreeFEM++, GetFEM++ [6, 7], and Comsol. But in this research, we used COMSOL® software because for optical device, the simulation result is close to the measured result.

The structure of waveguide in 2D that is shown in figure 1 and figure 2 show the 3D structure of waveguide. The main part was the core. The material of core was PMMA and the substrate material was silica glass. The analyte for sensing area was adjusted from refractive index 1.333 until 1.480. The core was described as having width (wcore) and height (hcore) and a refractive index (ncore). The refractive index 1.333 was illustrated some water and the refractive index 1.480 was same with ncore. The ammonia was described by refractive index 1.3334 until 1.480. The dimension of substrate in this simulation was 30 µm. The wcore and hcore were varied from 1 to 10 µm in steps of 1 µm. Dimensions of area for analyte was 30 µm in simulations.

The unit of electric field is V/m. Therefore, the dimensions can affect the electric field of waveguide. The optimum dimensions of core could be known by simulations. We simulated the model use FEM in COMSOL®. In this software, we employed RF Module, which combines the optics and photonics interfaces. The material properties used in the study are shown in table 1. The material properties in table 1 are valid for wavelength 1.55 µm, which is in the infrared region where most of the fibre optic communications operate [7, 8].

In this study, to investigate the dependence of the waveguide performance on the core dimensions, we used a modal analysis and the associated parametric sweep. The core dimensions were varied from 1 to 10 µm in step of 1 µm. This is the recommended range of core dimensions for the transmission wavelength at 1.55 µm [9]. The various values of core dimensions could determine the corresponding electric field intensities and effective refractive indices. A standard meshing tool was used with the mesh setting at physics–controlled mesh and element size set to “finer”. Figure 3 shows the meshed geometry of the waveguide cross section in 2D.

3. Results and Discussion
The first part of the modal study was the parametric analysis, which is the effect of core dimensions on the electric field intensities that propagates from the core into the analyte and substrate. The core dimensions were varied from 1 to 10 µm in step of 1 µm. The variation of electric field intensities propagating from the core into the analyte and substrate region was determined, as shown in figure 4.
Figure 4 shows the variation of electric field intensities from the core into the analyte and substrate region. From figure 3, the electric field intensities for all studied core dimensions fall to zero beyond the core dimensions. However, the electric field intensities on the core dimensions for 1 µm and 2 µm could be not shown here.

From figure 4, for the core dimension of $w_{core}$ 3 µm and $h_{core}$ 3 µm have the highest electric field

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**Table 1.** Material properties used in this study.

| Material     | Refractive Index |
|--------------|------------------|
| PMMA         | 1.48 (Core)      |
| Silica Glass | 1.45 (Substrate) |

**Figure 3.** Structure of the finite elements in COMSOL® for simulated waveguide.
at the centre of the core \((1.8 \times 10^7 \text{ V/m})\) while for core dimension of \(w_{\text{core}} 10 \mu\text{m} \) and \(h_{\text{core}} 10 \mu\text{m}\) have the lowest electric field intensity at the centre of the core \((7.7968 \times 10^6 \text{ V/m})\). For core dimension between 3 and 10 \(\mu\text{m}\), the electric field intensity at the centre of the waveguide decreases. However, while for the \(w_{\text{core}} 1 \mu\text{m} \) and \(h_{\text{core}} 1 \mu\text{m}\), there was no electric field intensity at the centre of core \((0 \text{ V/m})\). In addition, core dimension with \(w_{\text{core}} 2 \mu\text{m} \) and \(h_{\text{core}} 2 \mu\text{m}\) made the electric field intensity not focus at the centre of waveguide. This is because both dimensions were not recommended for single mode. As the dimensions of the core increased, the electric potential gradient reduced. Figure 5 and figure 6 show the electric field intensity using the Mode Analyses study from COMSOL® for the meshed structure in figure 2. From figure 5, the waveguide with dimensions of 3 \(\mu\text{m}\) does not confine all the energy within the core. This penetration of low-order and high-order modes into the analyte and substrate region indicates that some parts of electric field are refracted out of the core.

The refracted modes may become trapped in the analyte and substrate due to the thickness dimension of the analyte and substrate region. The trapped modes in the analyte and substrate region are called outer modes. As the core and the outer modes travel along the waveguide, mode coupling occurs. Mode coupling may occur when any two modes exchange power and this result in the loss of power from the core mode(s). As a result, energy may leak deep into the analyte or substrate, leading to substantial power losses especially in short waveguide [9,10]. On the other hand, a waveguide with \(w_{\text{core}}\) and \(h_{\text{core}}\) of 10 \(\mu\text{m}\), while it confines all the energy in the core, it also confines a substantial amount of weak fields within the core and hence reducing the peak intensity at the centre of the core (see figure 5). Figure 6 shows the fundamental mode of electric and magnetic fields for core dimensions of 3 and 10 \(\mu\text{m}\). Figure 7 confirms the leakage of energy from the core into the analyte and substrate region.

**Figure 4.** E-field intensities for various core dimensions.

**Figure 5.** 2D Electric field distribution for \(w_{\text{core}} 3 \mu\text{m} \) and \(h_{\text{core}} 3 \mu\text{m}\).
The maximum electric field intensity was achieved at \( w_{\text{core}} \) was 3 \( \mu \)m and \( h_{\text{core}} \) was 3 \( \mu \)m. The waveguide with \( w_{\text{core}} \) 10 \( \mu \)m and \( h_{\text{core}} \) 10 \( \mu \)m give the minimum electric field intensity. The highest electric field intensity shows the sensitivity of the sensor. As the dimensions of the core increased, the sensitivity reduced. Therefore, the most sensitive waveguide is achieved at \( w_{\text{core}} \) 3 \( \mu \)m and \( h_{\text{core}} \) 3 \( \mu \)m. For sensor applications, besides the sensitivity, the linearity is needed. Simulation of the linearity was conducted using parametric sweep on COMSOL for given refractive index of analyte that varies from 1.333 until 1.480. Further, the change in electric field could be seen. Figure 9 shows the change in electric field for 3 \( \mu \)m until 10 \( \mu \)m.

From figure 9, all dimensions of waveguide the electric field intensity tends to decrease as refractive index increase. For 3 \( \mu \)m and 4 \( \mu \)m, electric field increase at some points. This is probably due to error of measurement. The decrease of electric field falls while the refractive index changes from 1.453 to 1.493 for all dimensions waveguides. This happens because the refractive index analyte get near to \( n_{\text{core}} \), thus the electric field intensity decreases.

The optimum dimension for \( w_{\text{core}} \) and \( h_{\text{core}} \) is 5 \( \mu \)m. This dimension gives no noise and more sensitive than that over 5 \( \mu \)m. From figure 10, the core dimension at 5 \( \mu \)m shows linear decrease of electric field intensity.
Figure 9. Electric field distribution for 3 µm until 10 µm with the various refractive indexes.

Figure 10. Electric field distribution for 5 µm with the various refractive indexes.

4. Conclusions
The optimum dimension of waveguide for chemical sensor applications was successfully analysed using the FEM in COMSOL Multiphysics®. The higher value of electric field was achieved when the width and height of core is small. However, small core shows less linearity of electric field as a function of refractive index of analyte. Opposite trend happens for high dimensions of core. The results show that core dimensions at 3 µm gives the most sensitive sensor but less linearity and core dimension 10 µm has higher linearity but less sensitivity. The optimum dimensions of waveguide for sensor applications with moderate sensitivity and linearity is achieved at core width 5 µm and core height 5 µm. Therefore, the optimum dimensions of waveguide for ammonia sensor applications are 5 µm width of core and 5 µm height of core.

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