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# Determining Caffeine Concentration in Aqueous Solutions Using a High-precision Position-sensor-detector-based Measurement System

Yen Liang Yeh,* Wei Kai Xu, and Zong Han Li

Department of Mechanical Engineering, National Chin-Yi University of Technology, Taichung 411030, Taiwan, R.O.C

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We investigated the effect of caffeine concentration on the refractive index of aqueous solutions using a high-precision measurement system equipped with a position sensor detector. Experimental results indicated that the caffeine concentration directly affects the deflection distance. This deflection distance serves as the basis for determining the refractive index of the mixture solution. As the caffeine concentration of the mixture solution increases, the refractive index increases. In this study, the caffeine concentration of a mixture was 4%, and the refractive index was 1.3437. Thus, the caffeine concentration of a mixture can be determined on the basis of its refractive index.

## 1. Introduction

Liquid concentration can affect the physical properties of optical systems. The accurate measurement of liquid concentration often necessitates the use of expensive high-performance liquid chromatography devices. Light is refracted when it passes through different liquid media, which may have different refraction angles that can be used to distinguish them. In 1975, Grange *et al.*(1) used optical principles to measure the refractive index of liquid mixtures. In 1995, Docchio *et al.*(2) used a position sensor detector (PSD) to measure changes in refractive index, which corresponds to different liquid concentrations. In 1997, Feng *et al.*(3) used a heterodyne polarimeter to measure the optical rotation phase change caused by laser light passing through glucose solutions of various concentrations. Ghosh(4) performed optical measurement to determine the refractive properties and dispersion equation coefficients of birefringent materials using optical techniques. In 2007, Yeh *et al.*(5) measured the refractive index and thickness of birefringent materials using the changes in the light path caused by different refractions of the interferometer. They set up a high-precision measurement scheme by using the changes in the length of the light path in the interferometer for light that passes through a medium. These path length changes reflect different optical path lengths. Therefore, the refractive index and thickness can be effectively obtained. Different optical media have different

*Corresponding author: e-mail: ylyeh@ncut.edu.tw
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optical properties. From these properties, the difference in alcohol concentration in aqueous solutions can be determined. Therefore, we performed optical characteristic measurement to discriminate between liquids with various alcohol concentrations. Concentration changes are correlated with changes in light refraction. In 2008, Yeh and Lin[6] used an interferometer to measure changes in light paths, subsequently applying this approach to determine the alcohol concentration. In the same year[7,8], interferometry was used to measure changes in glucose concentration. In 2008, Yeh *et al.*[9] used a PSD to measure both the refractive index and thickness of wave plates. In a separate experiment in the same year, Yeh *et al.*[10] used both an interferometer and a PSD to simultaneously measure the thickness and refractive index of birefringent wave plates. In 2009, Yeh *et al.*[11] used a PSD to measure the alcohol concentration, augmenting its precision with interferometric corrections. By 2014, Yeh[12] had expanded research to include interferometric measurements of concentrations in methanol and ethanol mixtures. In another experiment in the same year, Yu *et al.*[13] controlled and stabilized the wavelength and power of laser emission. They used a compact, flow-through fiber-optic attenuated total-reflection sensor with a large optical sensing length for glucose level determination. In 2016, Lin[14] implemented high-resolution total-internal-reflection interferometry for measuring the refractive index of solutions by combining the advantages of both common-path and heterodyne interferometries. In 2022, Zhou *et al.*[15] set up a nanosensor consisting of a metal–insulator–metal waveguide with a rectangular root and a double ring with a rectangular cavity. This nanosensor was intended to detect the hemoglobin concentration in the blood. Because it can effectively measure the refractive index of objects, we used a PSD to measure the effect of caffeine concentration on the refractive index of liquid mixtures.

## 2. Experimental Setup

In this experiment, we used a laser and a PSD to measure the concentration of liquid mixtures. The laser penetrated a quartz glass box, and then an optical position sensor sensed the displacement distance of the laser spot, as shown in Fig. 1. The laser first passes through the quartz glass box and then irradiates the PSD. The PSD senses the center position of the laser, converts it to a numerical value, and outputs it to a computer. The quartz glass box was mounted on a rotating platform that could rotate horizontally. This rotation altered the angle between the laser beam and the horizontal axis of the quartz glass box, leading to a deflection and horizontal displacement of the light spot on the PSD. The laser used in this experiment was the He–Ni laser Newport N-LHP-151, and the PSD used was SPOTANA-9S-USB-Low. A diagram of the physical setup of the experiment is shown in Fig. 2. The theory underlying this experiment is presented in the next section.

## 3. Theoretical Analysis

When the laser light is perpendicular to the quartz wall, the incident angle of the laser is zero. Under these conditions, the laser experiences no deflection as it penetrates through liquids with

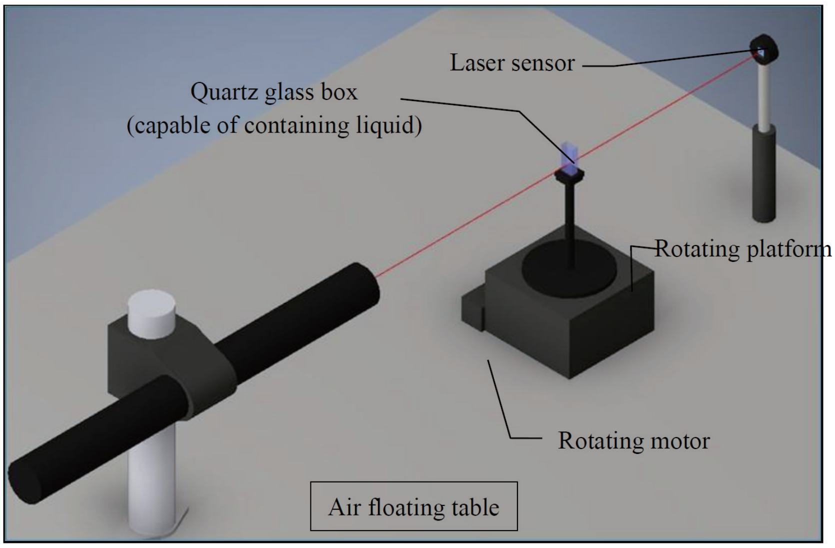


Fig. 1. (Color online) 3D schematic of optical measurement of liquid concentration.

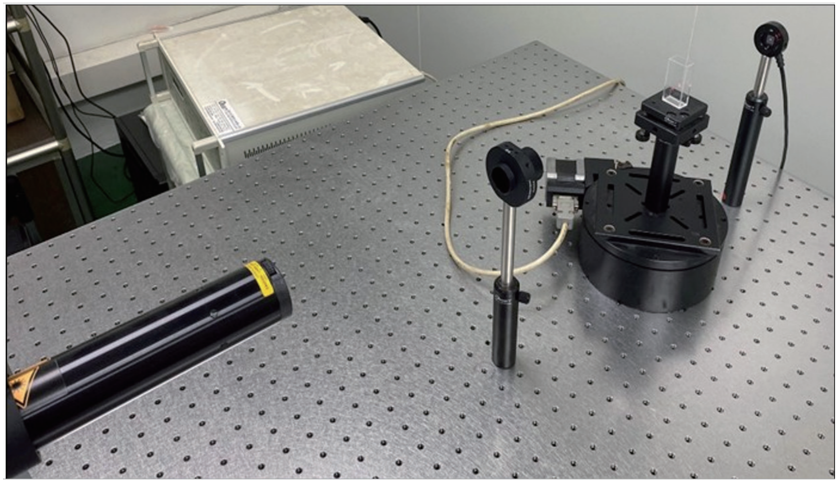

Fig. 2. (Color online) Position of mounted polarizer.

different refractive indices. Moreover, the position of the laser light spot on the sensor remains unchanged.

However, when the laser encounters the quartz wall at an incident angle of $\theta \neq 0$, the laser experiences deflection as it traverses liquids with different refractive indices. This deflection leads to the lateral displacement of the laser's path as it enters and exits the liquid medium. The lateral path resulting from the deflection path and the original path of the laser are parallel, as illustrated in Fig. 3. Consequently, the amount of deflection can be detected by the PSD.

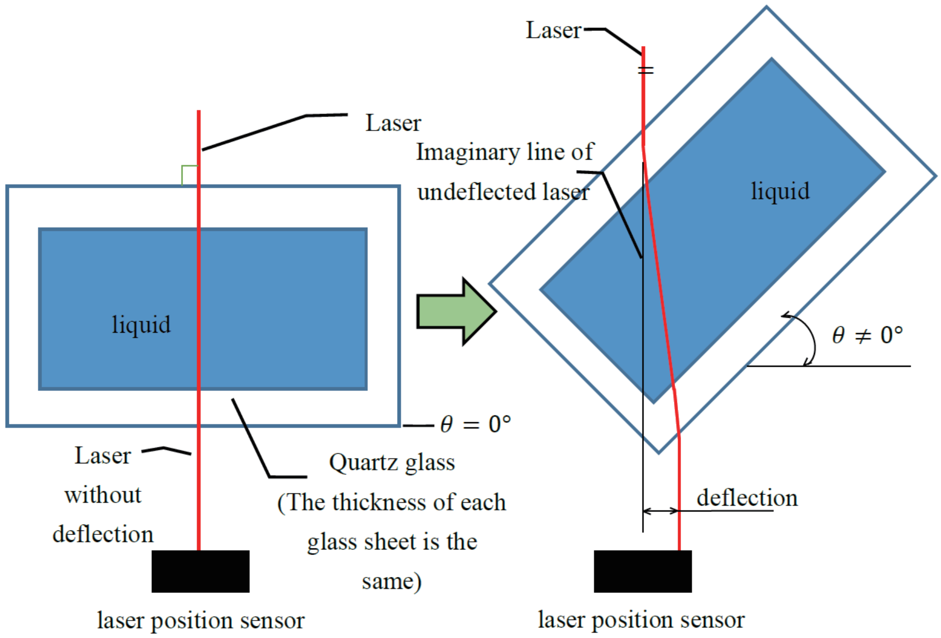


Fig. 3. (Color online) Schematic of laser penetrating quartz glass box and liquid.

## 4. Analytical Theory of Refractive Index

When the laser traverses the quartz glass box at incident angle $\theta$, its path is changed. This change in path contributes to the total deflection measured, as depicted in Fig. 4.

To convert this measured total deflection into a refractive index, variables such as the change in laser path angle, total deflection, the length of the light path, and dimensions of the quartz glass box are substituted into the appropriate formula.

The refractive index ($n_2$) of the liquid can be obtained using Snell's law expressed as

$$n_0 \sin\theta = n_1 \sin\varnothing_{d1}, \tag{1}$$

$$n_1 \sin\varnothing_{d1} = n_2 \sin\varnothing_{d2}, \tag{2}$$

where $n_0$ is the refractive index of air, $\theta$ is the incident angle of the laser, $n_1$ is the refractive index of quartz, $\varnothing_{d1}$ is the angle between the laser light path in quartz and the normal of the quartz wall, $n_2$ is the refractive index of the liquid, and $\varnothing_{d2}$ is the angle between the laser light path in the liquid and the normal of the quartz wall.

In this experiment, we used a laser of 632.8 nm wavelength. The refractive index of the laser at this wavelength in quartz was $n_1 = 1.543$, and the refractive index of the laser in air was $n_0 = 1$. The refractive index of the laser in the liquid was $n_2 = 1.33$. In Fig. 4, $X_1$ is the thickness of the

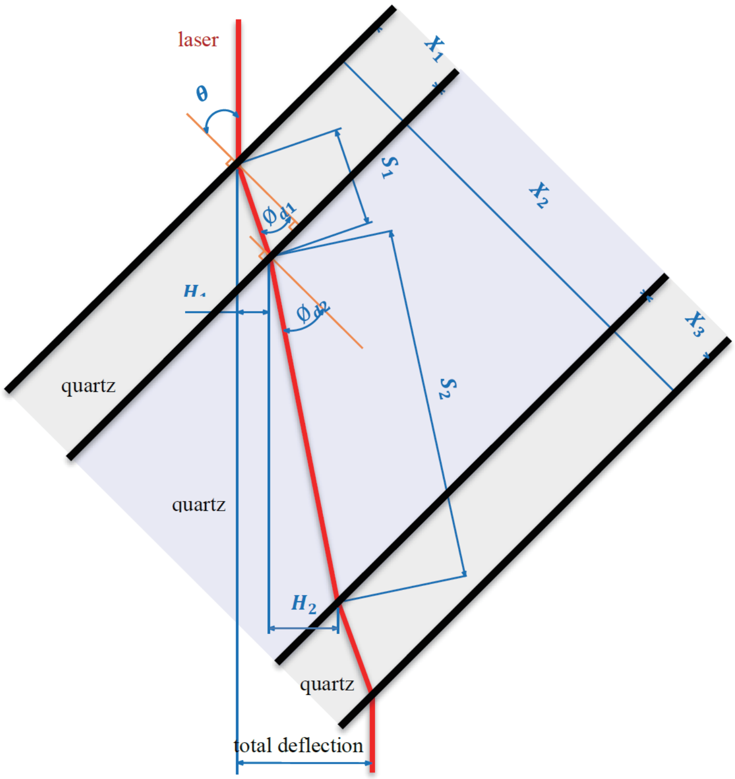


Fig. 4. (Color online) Schematic of laser path changes.

quartz wall, $X_2$ is the width of the quartz tank containing the liquid, and $X_3$ is the thickness of the opposing quartz wall. Additionally, $S_1$ is the laser path length in quartz and $S_2$ is the path length of the laser in the liquid. $H_1$ is the laser deflection distance in quartz and $H_2$ is the laser deflection distance in the liquid. $\theta$ is the angle at which the laser enters quartz from the air. $\emptyset_{d1}$ is the angle between the laser and the normal in quartz, and $\emptyset_{d2}$ is the angle between the laser and the normal in the liquid.

To calculate the refractive index ($n_2$), determining the angle ($\emptyset_{d2}$) between the laser light path in the liquid and the normal of the quartz wall is crucial. The formula used for this calculation is

$$\emptyset_{d2} = \tan^{-1}\left(\frac{\sin\theta - \dfrac{H_2}{X_2}}{\cos\theta}\right). \tag{3}$$

The refractive index ($n_2$) of the liquid is determined from the total laser deflection, which is detected by the PSD. This total deflection includes the deflection occurring in the quartz wall and that occurring in the liquid within the quartz tank.

Because the thickness of the walls of the quartz glass box is uniform and the laser must pass through two such walls, the deflection produced by quartz is regarded as twice the deflection distance ($H_1$) of the laser in a single quartz wall. When no liquid is present in the quartz tank ($H_2 = 0$), $2H_1$ can serve as a direct measure of the deflection.

Subtracting the deflection of the two quartz walls ($H_1$) from the total deflection yields the deflection specific to the liquid ($H_2$). The formula for this calculation is

$$H_2 = \text{total deflection} - 2H_1 . \tag{4}$$

To calculate the refractive index ($n_2$) of the liquid, the width ($X_2$) of the quartz tank containing the liquid is required. The formula to obtain $X_2$ is

$$X_2 = \frac{1}{S_2 \times \cos \varnothing_{d2}} . \tag{5}$$

The length of the laser's light path through the liquid mixture ($S_2$) can be obtained as

$$S_2 = \frac{H_2}{\sin\left(\theta - \varnothing_{d2}\right)} . \tag{6}$$

To ascertain the thickness of the quartz wall ($X_1$), the formula used is

$$X_1 = \frac{1}{S_1 \times \cos \varnothing_{d1}} . \tag{7}$$

The length of the laser's path in the quartz wall ($S_1$) can be calculated as

$$S_1 = \frac{H_1}{\sin\left(\theta - \varnothing_{d1}\right)} . \tag{8}$$

When the quartz tank is empty ($H_2 = 0$), the total deflection is $2H_1$ and can be directly measured. The refractive index of the laser in quartz was already established as $n_1 = 1.543$.

## 5. Quartz Tank Geometry Measurement

The laser entered the quartz glass at an incident angle of $\theta = 30°$. Angles exceeding 30° resulted in the lateral displacement of the laser beyond the range of the PSD. Angles below 30° yield less accurate measurement results. With an empty tank, the total deflection was $2H_1 = 484.1$ μm, making the deflection $H_1 = 242.05$ μm.

From Eqs. (1) and (2), an angle of $\varnothing_{d1} = 18.91°$ was obtained. Equation (6) yielded the path length $S_1 = 2516$ μm for the laser in the quartz wall. Equation (5) yielded the thickness of the quartz wall as $X_1$ = 1190 μm. Given the deflection distance in the wall of $2H_1$ = 484.1 μm, known laser refractive indices of $n_0$ = 1 for air and $n_2$ = 1.33 for water, and an incident angle $\theta$ = 30°, the width of the quartz tank containing the liquid was calculated. When the tank was filled with water, the total deflection was 2199.63 μm; this total deflection was deducted from the deflection distance $2H_1$ of the laser in the two quartz walls. The deflection distance of the water was $H_2$ = 1715.53 μm. From Eq. (3), the angle $\varnothing_{d2}$ = 22.08° was obtained. Substituting this angle into Eq. (6) gave the length of the laser path ($S_2$ = 12454 μm) in the liquid. Further substitution of $S_2$ into Eq. (5) yielded the width ($X_2$ = 11540 μm) of the quartz tank containing the liquid.

## 6. Experimental Results and Discussion

The liquid used in this experiment was a mixture of caffeine powder and water. The maximum detectable power that could be detected by the laser light sensor used was 2.93 mW. In the experiment, the laser entered the quartz glass at an incident angle of $\theta$ = 30°.

### 6.1 Experimental sample design

For a caffeine and water mixture, the caffeine concentration in aqueous solutions is expressed in weight percentage as follows.

Step 1: Weigh an empty measuring cup.
Step 2: Add transparent crystalline caffeine powder (99% purity, Alfa Aesar) to the measuring cup and record the weight.
Step 3: Dissolve the caffeine powder in 50 mL of hot water and allow the solution to cool to room temperature.
Step 4: Calculate the weight percentage of the caffeine in the aqueous solution.

### 6.2 Experimental measurement and analysis

We examined the effect of laser power on the deflection distance in liquid measurements. For this purpose, the deflection distances of lasers of various powers in water were measured. The findings revealed that laser power has a minimal effect on the deflection distance in water, as depicted in Fig. 5. The average deflection distance recorded in these experiments was 1504.43 μm.

The effects of laser power on the deflection distance in quartz were determined by using lasers with powers of 0.66 and 2.49 mW. The results also indicate a minimal effect of laser power on deflection distance, as depicted in Fig. 6.

We also explored how the caffeine concentration affected the laser's deflection distance in the liquid under ambient-light-free conditions. The data revealed a positive correlation between the caffeine concentration and the deflection distance, as depicted in Fig. 7, where the values correspond to the refractive indices displayed in Fig. 8.

In this experiment, we revealed that higher caffeine concentrations led to greater refractive indices, as shown in Fig. 8. A substantial change in refractive index occurred between caffeine

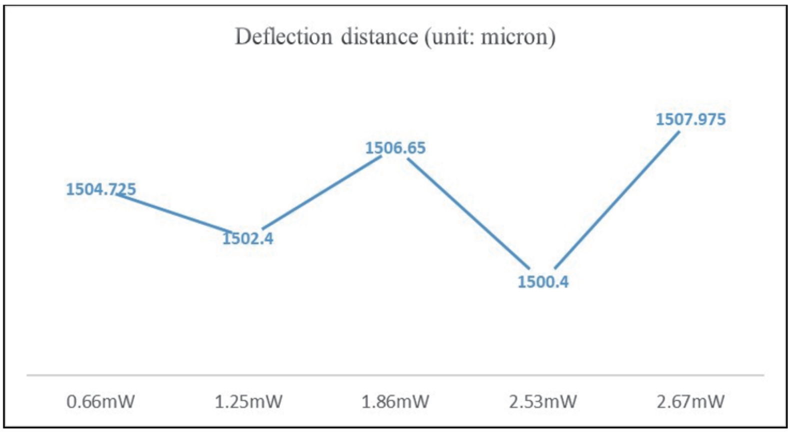


Fig. 5. (Color online) Deflection distance of liquid for lasers with various power settings, determined using a polarizer.

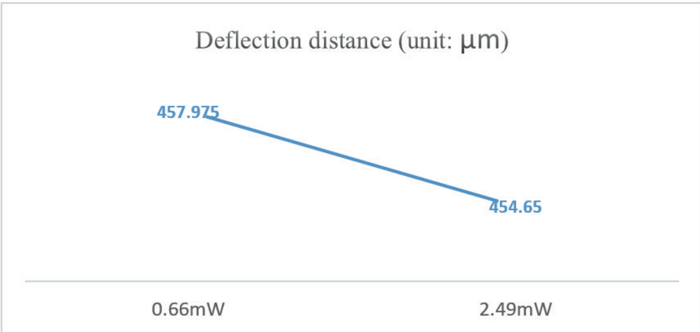


Fig. 6. (Color online) Deflection distance of quartz measured with different laser power settings.

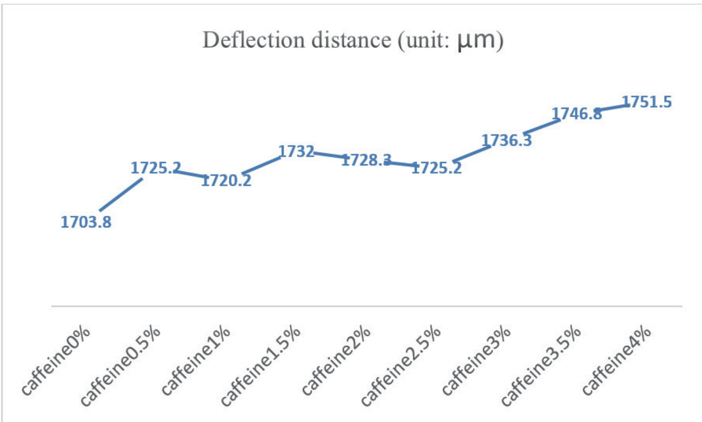


Fig. 7. (Color online) Laser deflection distance in liquid without ambient light.

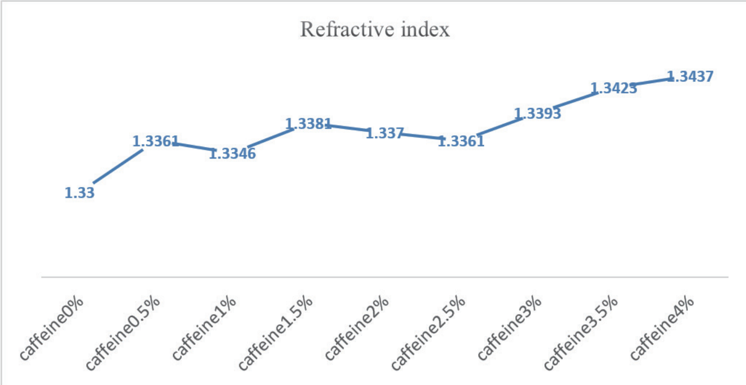


Fig. 8. (Color online) Refractive index of laser in liquid without ambient light.

concentrations of 0 and 0.5%. However, this change in refractive index was not statistically significant. As the caffeine concentration was increased from 0 to 4%, the refractive index increased from 1.33 to 1.3437. At caffeine concentrations exceeding 4%, the laser could not penetrate the mixture.

## 7. Conclusions

The caffeine solution used in this experiment was transparent and colorless, as were the caffeine crystals themselves. This experiment revealed that at concentrations exceeding 4%, caffeine is not fully soluble in water at room temperature; therefore, the experiment was restricted to a caffeine concentration range of 0 to 4%. Analysis indicated that higher caffeine concentrations modestly increased the refractive index. The results indicate a direct correlation between caffeine concentration and refractive index, albeit a moderate one. At a caffeine concentration of 4%, the refractive index was 1.3437. These findings suggest that changes in refractive index can serve as an indicator for determining a mixture's caffeine concentration.

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## About the Authors

**Yen-Liang Yeh** received his B.S., M.S., and Ph.D. degrees in mechanical engineering from Far East University in 1992, National Taiwan University of Science and Technology in 1998, and National Cheng Kung University in 2001, respectively. He is a professor with the Department of Mechanical Engineering, National Chin-Yi University of Technology. His research interests include mechanisms, CAE, structure analysis, optical measurement, nonlinear dynamics, and power systems. (ylyeh@ncut.edu.tw)

**Wei Kai Xu** received his B.S. degree in mechanical engineering from National Chin-Yi University in 2023, where he is also currently pursuing his M.S. degree in mechanical engineering. His research interests include mechanisms, CAD, structure analysis, optical measurement, and fluid mechanics. (g27510937@gmail.com)

**Zong Han Li** received his B.S. degree in mechanical engineering from National Chin-Yi University in 2023, where he is also currently pursuing his M.S. degree in mechanical engineering. His research interests include mechanisms, CAE, structure analysis, optical measurement, and institutional design. (1234484abc@gmail.com))