Near infrared light path simulation in a liquid bottle

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Introduction

Liquid explosives have recently been used in terrorism,[1] for example in the 2006 transatlantic aircraft plot in London. Liquid explosives and their raw materials can be hidden in bottles disguised as drinks. It is therefore important to scan the contents of bottles. A new instrument system using NIR has been developed for the detection of liquid explosives in bottles.[2] This instrument can scan liquids from the outside of the bottle instantly.

The NIR interactance method was used in the instrument shown in Figure 1. There were optical fibre bundles underneath the target bottle. A ring-shaped fibre bundle was connected to a light source and a central fibre bundle was connected to a spectrometer. Irradiation and detection of NIR light are simultaneously beneath the bottle. The light propagates throughout the bottle, reflecting and refracting at the various interfaces; a fraction of the light returns to the detector at the base. The measurement was performed at the base of the bottle to avoid labels which are generally wrapped around the sides.

This kind of instrument was designed to be used in public spaces where many people gather (for example airports, train stations and bus terminals). Many kinds of bottles are brought to these places. There are many unique shapes, colours and capacities. It is necessary to gain enough energy efficiency for reliable scanning of various bottles. Visualising light paths helps to optimise the placement of the light source and the detector. This is very useful for the design of optical systems requiring high detection efficiency.

One of the methods to visualise light paths is to add a scattering material to the liquid and observe the scattered light paths. This method is effective for directional light. However, it is not effective when a wide-angle source is used or the light propagates in a complex manner. Also, additional scattering material influences the light paths. Another visualisation method is light path simulation. This does not have the problems associated with adding a scattering material. Additionally, it is also possible to calculate the irradiance flux at the detector. In this study, the light paths in a bottle of liquid irradiated by an interactance system were visualised and analysed using light path simulation.

Materials and Methods

There were two steps for the light path simulation - modelling and configuration. For the modelling step, all parts of the bottle and the optical system were designed including the bottle, cap, and light source. In the configuration step, the optical properties of the parts and the parameters of the simulation were configured. The simulation was executed after the modelling and configuration.

Modelling

A 3D-CAD program, “Solid Works”(Dassault Systemés SolidWorks Corp., Paris, France), was used for modelling. A simple bottle model is shown in Figure 2. It was based on a PET bottle with a volume of 500 ml. It had a flat base and a round upper body. The top was covered by a cap and the bottle included liquid. The light source area was a ring shape and the detection area was circle with a diameter of 5 mm. These were placed concentrically under the bottle.

Configuration

The features of the bottle were as follows:
- The refractive index of the bottle was 1.58.
- The optical properties of the bottle were non-absorption and non-scattering.
- The surface had a character of specular reflection.
- The cap had the property of completely Lambertian reflection.
- The property of the liquid was set to water.

The features of the light source were as follows:
- The light source had a Gaussian distribution (the half-angle at half-maximum was 25 degrees and the half-angle was 50 degrees.)

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- The light wavelength was 600 nm. Although not in the NIR range, this wavelength was selected because the refractive index of water at 600 nm is almost equal to that in SNIR[3] and the effect of absorption or scattering could be removed for a simple simulation.

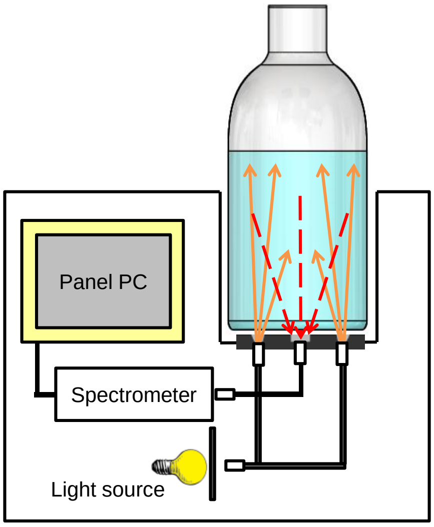

Figure 1. Schematic diagram of the bottle scan system.

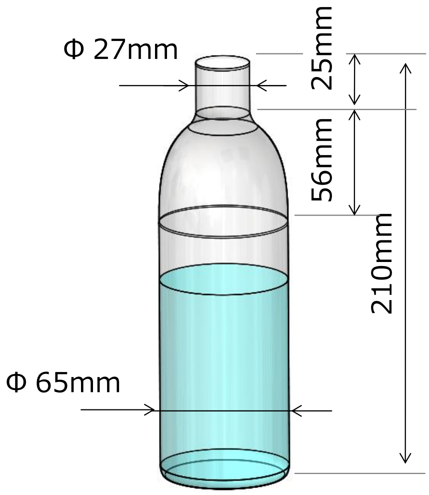

Figure 2. Simulation model of a bottle.

Simulation

A light path simulator, "OPTISWORKS"(OPTIS Corp., La Farléde, France) was used for this simulation. Optical-geometrical phenomena, absorption and scattering were simulated by the Monte Carlo Method. Finite element analysis was used for calculation. Discrete light paths were used instead of continuous light in the simulation. The outline of the simulation was as follows:

- A light path was irradiated from the light source at random.
- The light paths propagated straight and decayed in power due to the liquid absorption.
- The light paths were reflected or transmitted based on Fresnel's law at the interfaces between two materials.
- The simulation of each light path was terminated either when it returned to the detection area, when it left the bottle, or when the power fell below a certain threshold.
- A predefined number of light paths were irradiated consecutively.
- Finally, the power of light reaching the detection area was integrated.

The number of irradiated light paths ranged from 2×10^7 to 6×10^7 so that the number of light paths that reached the detector was more than 10^4. The liquid level was changed from 50 mm to 170 mm and the light paths were simulated for each level. The length of each light path was calculated and the distribution analysed.

Results and Discussion

Figures 3a, 3b and 3c show the irradiated light, detected light and histograms of the path lengths for liquid levels of 50, 100 and 150 mm, respectively. Examples of irradiated light paths are shown in Figure 3. The light essentially propagated vertically. This model can be considered by dividing it into two parts; the upper part, occupied by air, and the lower bottle, occupied by liquid. In the upper part, most light passed out of the bottle. On the other hand, in the lower part, most light was reflected by total internal reflection at the bottle wall and was trapped. The light reaching the detection area at the centre of the base is shown in Figures 3a-2, 3b-2 and 3c-2. This is composed of light paths reflected from the liquid surface, the top of the bottle and the cap. Most of these light paths were reflected from the liquid surface or cap. When the liquid level was high, light paths were concentrated at the cap. Histograms of the pathlengths that reached the detection area are shown in Figures 3a-3, 3b-3 and 3c-3. The light was grouped by the light path length; each bar of the histogram indicates the number of light paths within a 1 mm range. The vertical axis is the intensity of light detected at the centre of the base of the bottle, normalised with respect to the total number of light paths. One group consisted of light with path lengths from 420 to 500 mm; these values were almost twice the height of the cap (210 mm) and most of light in this group reached the detection area by reflection from the cap. The contribution of this group increased with the height of the liquid. This is because light was trapped by the

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liquid. The other group was composed of light paths which were about twice the liquid level. It suggested that light in this group was reflected at the liquid surface once and returned to the bottom of the bottle.

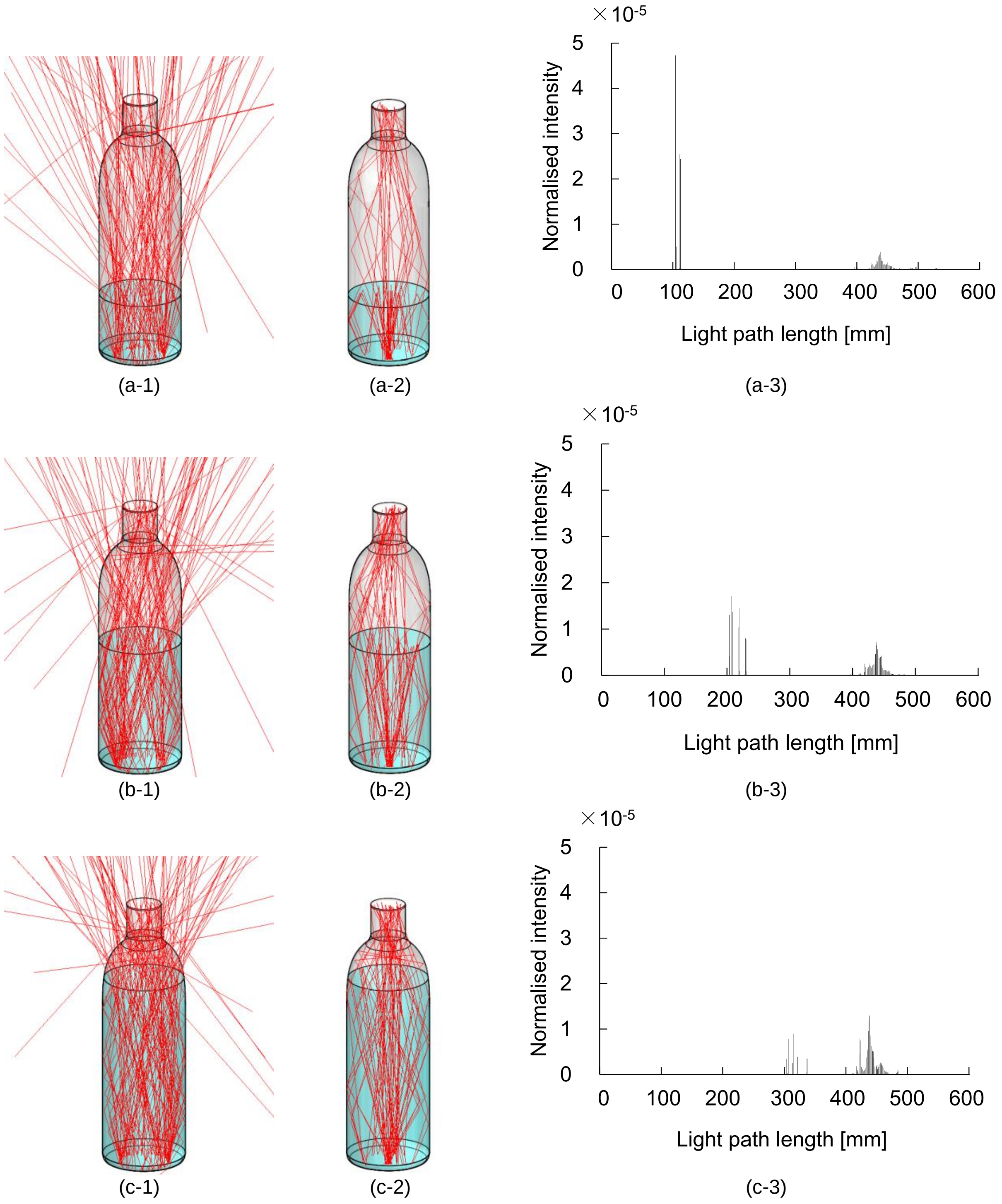

Figure 3. (1) Irradiated light, (2) detected light and (3) histograms of light path lengths for liquid levels of (a) 50, (b) 100 and (c) 150mm.

The normalised intensity of light that reached the detection area is shown in Figure 4. “Reflected at the cap” was defined as the intensity of light which reached both the cap and detection area. “Reflected at the liquid surface” was defined as the intensity of light which was not reflected at the cap but only at the liquid surface. “Reflected at the bottle” was defined as the intensity of other light paths reflected at the top of the bottle excluding the cap. Each group was divided by the total number of irradiated light paths for normalisation. Their values were less than 0.1%. As the liquid level was increased, intensity tended to increase. This was due to the light paths being focussed at the cap and reflected back to the detector.

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The normalised intensity is related to absorbance. Absorbance is defined as $A = \log_{10}(I_0/I)$ where I_0 is the reference intensity and I is the intensity of light passing through the material. In our case, the light paths passing through the liquid and reference, an empty bottle, were different, so I_0 could not be measured directly. Instead of I_0, we define I_0' the spectrum of the light source as the reference. Because the absorbance uses the log of I_0, and the second derivative is taken, using I_0' has no effect on the result. (I_0'/I) is the inverse of the normalised intensity in figure 4.

Figure 5 shows the relationship between the liquid level and average light path length which reached the detection area. The higher the liquid level was, the longer the average path lengths tended to be. The average length of the part of the path passing through the liquid was about twice the liquid level. This indicates that light travels vertically and was reflected directly back to the detector. According to the Lambert-Beer law, absorbance is proportional to the light path length. Therefore, the liquid level and the volume of the liquid can be estimated approximately from the absorbance.

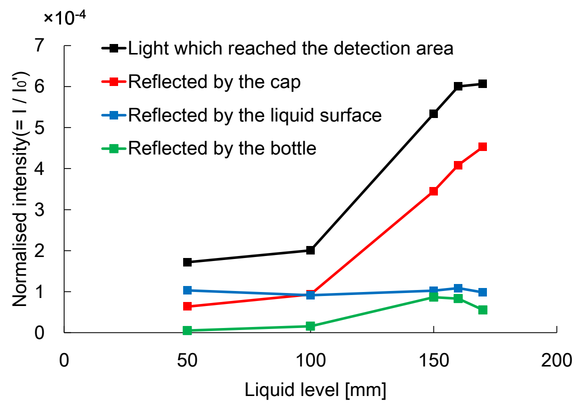

Figure 4. Normalised intensity of light that reached the detection area.

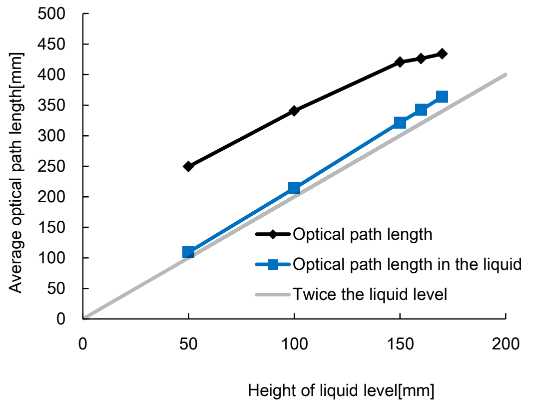

Figure 5 Average path lengths of light that reached the detection area.

Conclusion

Light distribution in a bottle in an interactance system was visualised using light path simulation. Irradiated light which reached the detection area was separated into two groups: one was composed of light reflected by the liquid surface and the other was composed of light which reflected at the top of the bottle, predominantly by the cap. As the liquid level was increased, the intensity tended to increase. The average light path length in the liquid was about twice the liquid level. It indicated that the liquid level and the volume of the liquid could be estimated approximately by the absorbance. Light path simulation was an effective tool for the visualisation of light paths and construction of optical systems.

The simulation showed that irradiated light propagated and was absorbed throughout the liquid in a bottle when it was irradiated from the bottom. This indicated that our instrument could scan and evaluate the liquid content in bottles.

Acknowledgements

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