Detection of Vinyl Chloride in environmental water samples

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Abstract

Abstract. write toward the end

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Abbreviations

VOC	Volatile Organic Compound
VC	Vinyl Chloride
PVC	Polyvinyl Chloride
GC	Gas Chromatography
GSC	Gas-solid Chromatography
GLC	Gas-liquid Chromatography
EHP	Environmental Health Perspectives

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Background

Humans produce waste, whether that is as an individual or on an industrial level. A lot of the waste that is being produced, end up in our water supply contaminating it. An example of a toxic waste product that can end up in the water supply is vinyl chloride *(VC)*, one of the primary areas VC is found is in the production of PVC. PVC plastic is used as pipes for plumbing, bottles, and more[3]. Vinyl chloride is a highly volatile compound which makes it both hard to detect, and making it more dangerous. This has created a need for a fast and simple solution for detecting the concentration of vinyl chloride in water samples.

This has led the company Water Care Guard *(WCG)* to develop an on-site lab kit that fits in a suitcase, which is able to test a water sample for the concentration of vinyl chloride amongst other substances.

This project is done in collaboration with Roana from SDU Nano Syd and Water Care Guard.

Problem

As it stands at the moment, when you want to detect vinyl chloride in water samples you use a method of analysis called *"Gas chromatographic (GC) analysis"*[2]. Gas chromatographic analysis is an analysis method in which the sample is being heated to the point of each component in the sample is being vaporized, where it then enters a column where the different components are being separated, such that it can be detected.[4] The process of sending a water sample to a laboratory and getting the measurements made, is time-consuming and expensive. It can take up to two weeks to get a water sample analyzed in a laboratory.[5] The solution with Water Care Guard, aims to reduce this time, by creating an onsite *laboratory kit*, where you can test the water sample. It is using the fact that the refractive index of the solution with added enzyme is dependent on the concentration of vinyl chloride in the solution. The refractive index can be determined using a spectrophotometer and a cuvette with a photonic crystal applied to one side.[1]

The main part of the project is going to be about building a database for different vinyl chloride concentrations and the refractive index shift for the corresponding vinyl chloride concentration. In addition, the data from the database should be analyzed to be able to get a prediction for the concentration of vinyl chloride in the solution based on the sample given.

The second part of the project is building a simplified user interface for the suitcase, which could be installed on a tablet in the suitcase or another display that the user can interact with. It could even be used on the smartphone of the user, or something else. This could be accomplished by making a dedicated app, or by having a website that is hosted on a computer in the suitcase, this would allow the user to access the user interface from either a tablet in the suitcase or from their computer or smartphone.

Timetable and milestones

The project is divided into 3 main parts:

- Building the database
- Analyzing the data
- User interface

The different parts are going to overlap, but it is primarily going to be in the order of the first part is focusing on building the database then about finding a way to analyze the data, and lastly building the user interface.
The project is divided up with the intention of spending 8 hours per day, 5 days a week on the project i.e. 40 hours a week.

Gantt chart

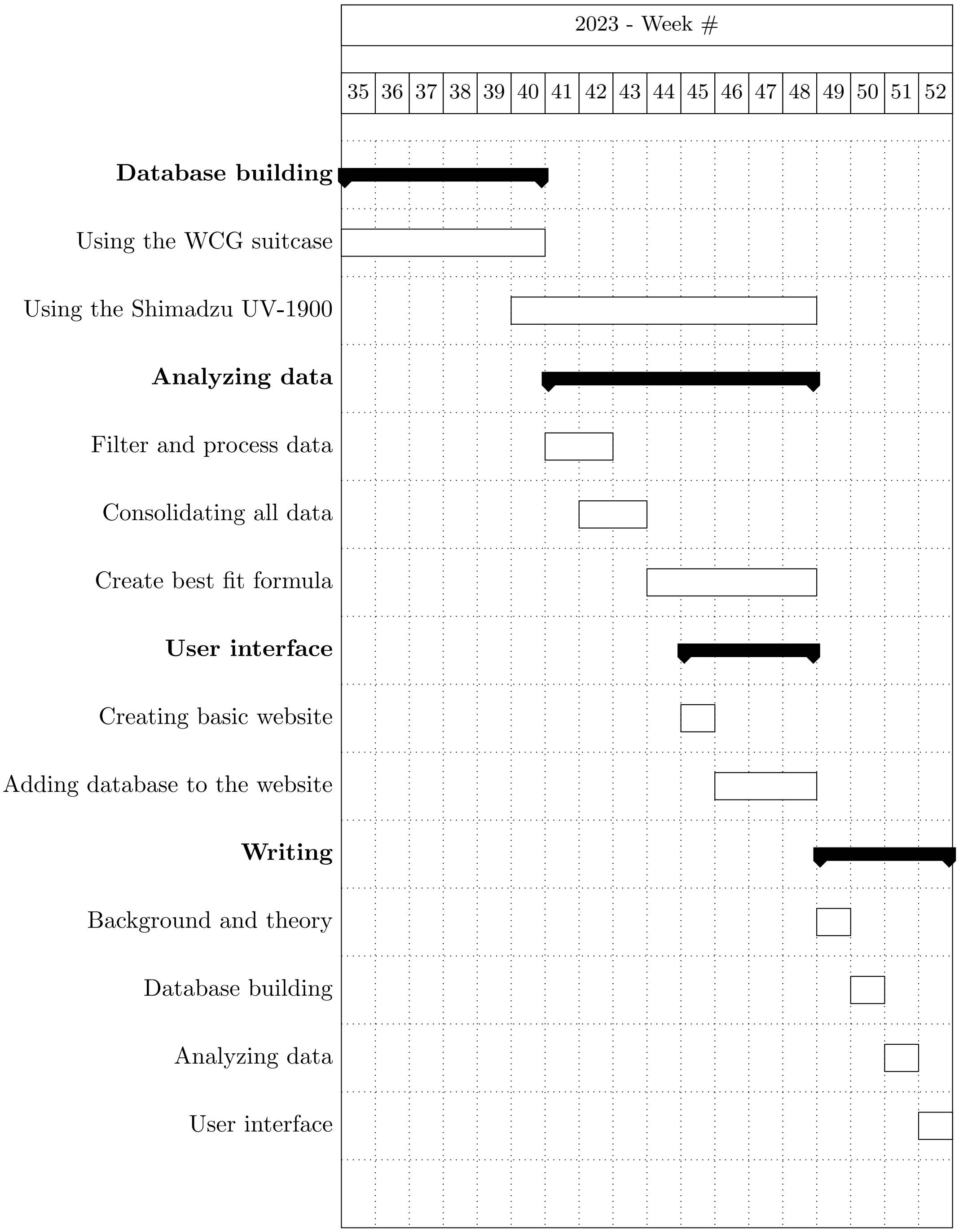

Figure 1: The timetable in a Gantt chart format, divided up in weeks

Risk assessment

The primary risk associated with the project is regards to dealing with the chemicals in making the measurements.

Issue	Who is involved	Impact/Probability	Mitigative actions
High volatility and toxicity of Vinyl Chloride. Working with the chemicals	Operator performing the measurements	High/High	Using: - labcoat - safety glasses - working in a fume hood

Table 1: The risk assessment table

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1 Introduction

1.1 Background

Humans have been producing waste for a long time, but as the materials that we use change so has our waste. In the early 20th century with the invention of fully synthetic plastic by the Belgian chemist Leo Baekeland in 1907[1], started a new type of anthropogenic pollution. One type of plastic known as Polyvinyl Chloride (PVC), which was first synthesized in 1872 by Dr. Eugen Baumann[2], it was first plastasized by Dr. Waldo L. Semon in 1926[3]. The introduction of plastics and especially PVC plastics, has introduced a new biproduct which is a highly toxic volatile organic compound (VOC), called Vinyl Chloride (VC). Vinyl chloride is a biproduct in the production of PVC plastics, from it being used as the main component in the production of PVC plastics. PVC plastics are used in a lot of different areas like construction piping, packaging, wires, toys, etc. in figure 1 some examples of PVC applications are shown.

Figure 1: Applications for PVC plastic. [4]

People can be exposed to vinyl chloride in different ways, through inhalating contaminated air, contaminated water etc. If vinyl chloride contaminate a water supply to a household, it can contaminate the air in the household leading to the inhabitants being exposed to vinyl chloride. [5] One of the main dangers with exposure to vinyl chloride is the increased risk of cancer, and in particular liver cancer.[5] In addition according to *"kemibrug.dk"*[1], vinyl chloride can also affect the central nervous system with symptoms like headache, dizziness, nausea and a possibility of loss of conscioiusness, as well as the inhalation the chemical is also easily absorbed through the skin which can lead to similar effects as of those from inhilation.[6]

At the moment the primary way to analyze whether there is vinyl chloride present in a water sample is through gas chromatography. According to an article from F.J Santos and M.T Galceran some of the advantages of gas chromatography are that is has a very high selectivity and resolution, making it easier to detect even small quantities of vinyl chloride in the sample, in addition GC has a good accuracy and precision.[7]

Gas chromatography is a physical process where a mixture of different substances are separated into their different parts.[8] There are two primary types of gas chromatography, gas-solid chromatography (GSC) and gas-liquid chromatography (GLC), in gas-solid chromatography it is about the absorbtion of the sample on the solid and with gas-liquid chromatography it is about the solubility of the sample to the liquid. [9] In the case of detecting the vinyl chloride it is GLC that is being used, since the sample to be tested for the concentration of vinyl chloride is usually water. According to the "Environmental Health Perspectives (EHP)" some of the areas that there have been shown high levels of VC are "soil, groundwater, aquifiers, and wells near landfill and industrial waste disposal sites"[10]. Gas chromatography works by having a sample that is to be analyzed, that is injected into a moving gas stream. It is then being carried down a column by a liquid with a low volatility, the sample is then separated into its different parts because the absorptivities and solubilities of the different parts differ making them arrive at different rates which makes it possible for the detector at the end to get a reading.[9] The process is illustrated in figure 2.

[1] A database for information regarding chemicals

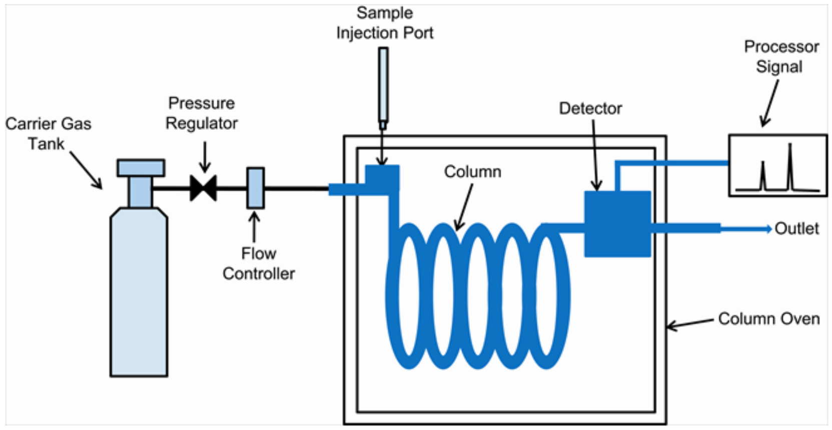

Figure 2: Schematic illustration of a gas chromatography system. [11]

A gas chromatograph is an expensive piece of laboratory equipment[12], in addition it can take up to two weeks to get a sample analyzed in a laboratory[13]. This is why there is a need to be able to get a faster on-site detection of vinyl chloride concentration in water samples. This is what the company Water Care Guard[2] is working towards, with their suitcase laboratory. Instead of using GC for detecting the vinyl chloride, it is using an enzymatic reaction between the vinyl chloride and an enzyme (Cytochromes P450), this enzymatic reaction changes the refractive index of the solution over time where the shift in the refractive index from the starting point is related to the concentration of the vinyl chloride in the solution.[14][15].

[2]https://www.watercareguard.com/

2 Theory

This section will be explaining the relevant concepts, for the method that is used for detecting vinyl chloride in the Water Care Guard suitcase.

2.1 What is ***Refractive index***?

The definition of refractive index from The Britannica Encyclopaedia is:

> "measure of the bending of a ray of light when passing from one medium into another"[16]

The refractive index is defined as the the sine of the angle of incidence to the sine of the angle of refraction.[16] Equation 1 shows how the refractive index is calculated as either the ratio of the sine of the angles or as the ratio of the speed of light in a vacuum (c) over the speed of light in the medium (v).[17] The angles, i and r are shown in figure 3.

$$n = \frac{\sin i}{\sin r} = \frac{c}{v} \tag{1}$$

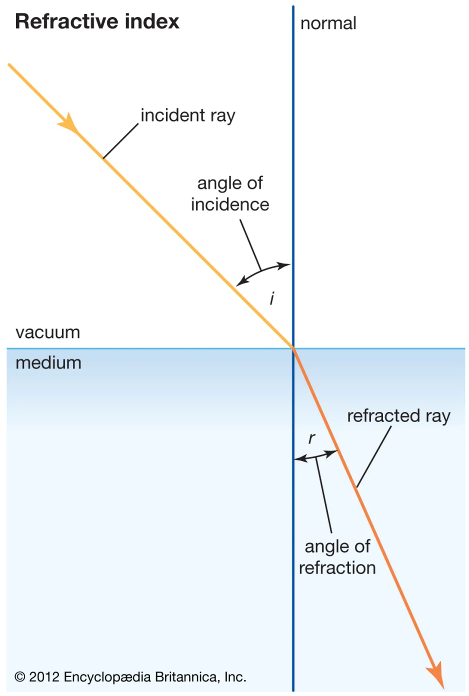

Figure 3: An illustration of refractive index[16]

2.2 The photonic cystals, a tool for measuring the refractive index

3 Building a database

3.1 Measuring vinyl chloride in a sample

3.1.1 General methodology

During the measurement gathering process, there was a procedure that was followed for all the measurements, it was adapted slightly depending on what instrument the measurement was done on. Firstly the instrument was turned, and proceeding with the steps only when the instrument had heated up. With the Water Care Guard suitcase or with the Ocean Optics UV-650 UV-VIS^{TM}, the heat up wait was a fixed 15 minute wait, because those instruments did not have a heating status indicator telling when it was finished heating up. On the other hand with the Shimadzu UV-1900^{TM}, there is a light on the front indicating the status, if it is yellow it is still heating and green when it is ready, this is indicated in figure 4.

(a) Shimadzu UV-1900 warming up indicator

(b) Shimadzu UV-1900 ready and done warming up

Figure 4: Shimadzu UV-1900 status indicator

After the instrument has heated up, a water reference measurement is then completed in the Spectroworks^{TM} software by Copenhagen Nanosystems

3.1.2 Measuring using the Water Care Guard suitcase

3.1.3 Measuring using the Shimadzu UV-1900 spectrophotometer

3.2 Problems

3.3 Data analysis

4 User interface

4.1 API Interface

4.2 Graphical User Interface

5 Conclusion

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6 Appendix