Simulating Experiments using a Comsol Application for Teaching Scientific Research Methods

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Abstract: For universities it is important to teach the principles of scientific methods as soon as possible. However, in case of performing experiments, students need to have some knowledge and skills before start doing measurements. In this case, Comsol can be helpfully by simulating the experiments before actual doing it. Especially the Comsol App can be very suitable because it provides a way for students playing with virtual experiments without almost any prior software (Comsol) experience. It is concluded that Comsol is very suitable for this type of education.

Keywords: Research, Methods, Comsol, Science, Education

1. Introduction

The scientific method requires techniques for investigating phenomena, acquiring new knowledge, or correcting and integrating previous knowledge [1]. The Oxford English Dictionary defines the scientific method as "a method or procedure that has characterized natural science since the 17th century, consisting in systematic observation, measurement, and experiment, and the formulation, testing, and modification of hypotheses " [2]. For universities it is important to teach the principles of scientific methods as soon as possible. However, in case of performing experiments, students need to have some knowledge and skills before start doing measurements. The paper presents an introduction of a first year course on scientific methods for building physics, a description of the experiment, the use of Comsol to simulate the experiment and how students learned from all this.

2. Summary of a first year course on scientific methods for building physics

In Table I a weekly schedule of the course is provided

<table>
<thead>
<tr>
<th>Topic (One each week)</th>
<th>Learning goals for Intermediate Test</th>
<th>Learning goals for Final Test</th>
</tr>
</thead>
<tbody>
<tr>
<td>Workshop &amp; assignment on: Literature study</td>
<td>Introduction of the project.</td>
<td>What are the key ingredients of scientific papers?</td>
</tr>
<tr>
<td>Workshop &amp; assignment on: Simulation</td>
<td>How to use FEM oriented simulation software? How to get data from the model?</td>
<td>Simulate the experiment using Comsol app.</td>
</tr>
<tr>
<td>Workshop &amp; assignment on: Data Analysis</td>
<td>How to visualize data? How to analyze data using basic statistical metrics?</td>
<td>Estimate the thermal conductivity and the accuracy using your simulation results of experiments</td>
</tr>
<tr>
<td>Workshop &amp; assignment on: Measurement</td>
<td>What are the key ingredients of scientific measurements</td>
<td>Estimate the thermal conductivity and the accuracy using your measurements</td>
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<tr>
<td>Doing experiments at the lab</td>
<td></td>
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<tr>
<td>Application of skills for final product</td>
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<tr>
<td>Application of skills for final product</td>
<td></td>
<td>Product delivery (Final paper)</td>
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</tbody>
</table>
The basic idea is to introduce four common research methods: Literature study, experiment, simulation and data analysis to first year students. The students use these methods to do research and write their first scientific paper. After the course, students have knowledge on:

- Science as a method of doing research
- The most important research methods for engineering such as: Literature study; Data analysis; Measurement and Simulation.
- Reading and reviewing scientific papers, assess the quality of report and papers
- Tools for data analysis: visualization techniques, regression, curve fitting
- Measurement accuracy, error estimations, sensor influence on process
- Simulation reliability, verification and validation

The assessment and grading is shown in Table II using rubrics:

Furthermore, the students gain experience by doing: A literature study; data analysis; measurement and simulation.

### 3. Description of the experiment

The experiment consists out of a well-insulated, lidless, box made of expanded polystyrene (EPS), in which a heat source is placed. A ventilation system is also installed in the box to ensure that the heat is evenly spread throughout the box’s volume. The heat source and ventilation system combined produce 41.3 W. A sheet of polymethylmethacrylate (PMMA)—of which the thermal conductivity is to be determined—is attached to the top of the box. The insulated box made of EPS has a thermal conductivity of 0.035 Wm⁻¹K⁻¹ ±0.001 Wm⁻¹K⁻¹. To determine the thermal conductivity of the sheet of PMMA using Fourier’s law of conduction, a heat flux sensor is installed. Furthermore, a sheet of polyvinyl chloride (PVC), with a thermal conductivity of 0.17 Wm⁻¹K⁻¹ ±0.02 Wm⁻¹K⁻¹, is attached onto the sheet of PMMA as a reference material to conduct the DTA-method. Additionally, several thermocouples are installed to measure the following temperatures:

- Air temperature inside the box (T_{ai})
- Surface temperature inside the box (T_{si})
- Temperature between the sheet of PMMA and the sheet of PVC (T_{mr})
- Surface temperature outside the box (T_{so})
- Surface temperature inside the heat flux sensor (T_{sih})
- Temperature between the sheet of PMMA and the heat flux sensor (T_{mh})
- Surface temperature outside the heat flux sensor(T_{soh}).

The EPS box has the following dimensions: a length of 600mm ±2mm, a width of 400mm ±2mm, a height of 190mm ±2mm and a thickness of 21mm ±1mm. The sheet of PMMA has a thickness of 10mm ±0.1mm and the reference sheet of PVC has a thickness of 4.1mm ±0.05mm as can be seen in Figure 1.
With this App the students are able to gain experience by doing virtual experiments. Moreover, the students simulate the output (time series) of the sensors including temperatures and heat fluxes. After the data analysis workshop, they are able to use these simulated data to calculate the objective parameter: the heat conduction coefficient of the sample and compare this with input value. With this procedure the students learn to verify both the simulation as well as the data analysis method.

5. Results
We refer to the Appendix where a first scientific paper of a representative student is provided.

6. Conclusions
For universities it is important to teach the principles of scientific methods as soon as possible. However, in case of performing experiments, students need to have some knowledge and skills before start doing measurements. In this case, Comsol can be helpfully by simulating the experiments before actual doing it. Especially the Comsol App can be very suitable because it provides a way for students playing with virtual experiments without almost any prior software (Comsol) experience. Students can learn from this, before doing the real experiment. For example: (1) Simulated sensor data provide a way to do data analysis in an early stage; (2) Studying the disturbances (systematic errors) of the process by placing sensors; (3) Design of the experiment and improvement of the expected sensor responses. The paper presents an introduction of a first year course on scientific methods for building physics, a description of the experiment, the use of Comsol to simulate the experiment and how students learned from all this. It is concluded that Comsol is very suitable for this type of education.

References
[1]. Goldhaber & Nieto 2010, p. 940
[2]. From the Oxford English Dictionary definition for "scientific".

Appendix
A representative output of the educational project: A first scientific paper of a student.
Abstract
This research study investigates three methods of measuring the thermal conductivity of PMMA. These three methods are: the DTA-method, the use of Fourier’s law with a heat-flux sensor and a computer software simulation. Before the experiment was conducted and the simulation run, the author investigated the various means of measuring a material’s thermal conductivity, as well as the limitations and advantages of each method.

The research experiment and computer simulation found that Fourier’s law remains the most accurate method of determining the thermal conductivity of PMMA, that the DTA-method may also be used with twice the level of inaccuracy. Finally, the simulation program, despite its practical advantages and removal of human calibration error, was the least accurate, though this was likely due to the elementary nature of the simulation itself.

The research concluded that, although Fourier’s law remains by far the most accurate of the three methods, that potentially the DTA-method and the simulation method may be improved with the use of a more precisely known reference material and the use of a more in-depth and comprehensive computer program.

Keywords: Thermal conductivity; PMMA; Fourier’s law; DTA-method; Comsol simulation

1. Introduction
In recent years both the effects and awareness of global warming have become increasingly prominent and, as a result, there has been an increasing effort by individuals, governments and corporations to do something about it. Furthermore, the building sector has been a major contributor to CO2 emissions, which itself is a significant contributor to global warming. A reduction in CO2 emissions may be achieved by insulating buildings more effectively, so that less energy is required when heating them up or cooling them down. Thermal conductivity therefore becomes a means of reducing CO2 emissions and, therefore, by assessing the conductivity of a particular material, one is able to more accurately determine its use as an insulating material.

The transfer of heat happens via three means; convection, radiation and conduction. Heat transfer via convection occurs in a fluid (that is; liquid or gas state) when particles move from a hotter, and therefore less dense region of a material, to a colder and denser region of material. Heat transfer through radiation demands no contact between the hotter and colder material, indeed, infrared radiation can be transmitted through vacuum. Finally, heat may be transferred via conduction, which shall be the research subject of this study. Conduction occurs when the molecules within a substance are heated, thereby having greater energy, which is subsequently transferred via the contact of the molecules themselves to other molecules within the substance.

Different materials used in the construction sector possess different levels of thermal conductivity. When the thermal conductivity of such materials is determined with greater accuracy, these materials may then be utilised more efficiently in order bring down the energy usage of the construction industry, as well as its products and services. The methodological choice in determining the thermal conductivity of a material is dependent upon the geometry of the material tested, as well as its dimensions and the magnitude of the expected thermal conductivity [1].

This study shall focus on polymethylmethacrylat (PMMA) and shall try to analyse the material in the most accurate manner to fulfil the research aim. The aim of this research study is to compare several methods of determining the thermal conductivity
of PMMA to ascertain which is the most accurate. For this research experiment, a sheet of PMMA is to be used with a thickness of 10mm. PMMA is a transparent thermoplastic synthetic polymer with an expectedly quite low thermal conductivity [2].

In the past, and especially throughout the 19th century, numerous researchers have investigated the thermal conductivity of several different materials. Around 1850 a new method was developed by the Scottish-born James David Forbes, a method entirely based on conduction. This method involved a bar, comprised of the material to be tested—being heated on one end and the temperature being measured on the opposite end. When this method is applied to materials with a relatively high thermal conductivity, the difference in temperature on the opposite end can be easily noted. For materials such as PMMA, which possess a relatively low thermal conductivity, this difference is more difficult to determine. However with the use of contemporary infra-red imaging, it is now possible to note even slight temperature differences. The infra-red method however, remains relatively inaccurate [3].

Around the same time as Forbes, Joseph Fourier was doing research to the same property. At the time that Fourier was conducting his experiments, no accurate equipment existed to measure the heat flux, and so—with a lack of proper measuring equipment—Fourier decided to conduct his research on a theoretical basis by mathematically deducing what would become known as Fourier’s law of conduction [4].

The differential scanning calorimetry (DSC) method was invented due to technological improvements in measuring equipment throughout the 1960s. This thermoanalytical technique, measures the difference in the amount of heat required to maintain a certain temperature within a sample and a reference material. These two measurements are proportionate to each other and, since the thermal conductivity of the reference material is already known, the thermal conductivity of the sample can be determined. The accuracy of the DSC-method generally falls within 10% of accuracy, as temperature sensors are not required. For sample materials such as PMMA this technique enables both an expedient and suitable method for determining a substances thermal conductivity [5][6].

A variation of this DSC-method is the differential thermal analysis (DTA)-method. Within the DTA-method, the thermal cycles that both the sample material and the reference material undergo are identical. Therefore, instead of keeping the temperature the same, the thermal cycle is now kept the same. The temperature difference between the sample and reference material is recorded and, using the proportionality of these two measurements, the thermal conductivity of the sample can be determined.

Subsequently, over the last few decades, computer simulations have become more complex and powerful and therefore are able to represent reality and real-life experiments in a more accurate manner. Research has been undertaken so that it is now possible for random microstructures to be entirely recreated digitally within a computer program, and therefore the thermal conductivity of various materials may be determined more accurately [7]. The complexity of these programs however means that they are generally less accessible, and therefore many researchers are forced to utilize more elementary computer programs in order to simulate a real-life experiment.

This study shall research the thermal conductivity of PMMA using Fourier’s mathematically deduced law of conduction, the DTA-method and the simulation software Comsol, comparing these methods in accuracy.

### Nomenclature

- **A** surface area in m²
- **C** calibration value in Wm⁻²mV⁻¹
- **d** thickness in mm
- **e** thermo-electromotive force in mV
- **q** heat flux density in Wm⁻²
- **Q** heat flux in W
- **R** thermal resistance in m²KW⁻¹
- **T** temperature in °C
- **λ** thermal conductivity in Wm⁻¹K⁻¹

### 2. Methodology

#### 2.1 Materials

The experiment consists out of a well-insulated, lidless, box made of expanded polystyrene (EPS), in which a heat source is placed. A ventilation system is also installed in the box to ensure that the heat is evenly spread throughout the box’s volume. The heat source and ventilation system combined produce 41.3Js⁻¹. A sheet of polymethylmethacrylat (PMMA)—of which the thermal conductivity is to be determined—is attached to the top of the box. The insulated box made of EPS has a thermal conductivity of 0.035Wm⁻¹K⁻¹ ±0.001 Wm⁻¹K⁻¹. To determine the thermal conductivity of the sheet of PMMA using Fourier’s law of conduction, a heat flux sensor is installed. Furthermore, a sheet of polyvinyl chloride (PVC), with a thermal conductivity of 0.17Wm⁻¹K⁻¹ ±0.02 Wm⁻¹K⁻¹, is attached onto the sheet of PMMA as a reference material to conduct the DTA-method. Additionally, several thermocouples are installed to measure the following temperatures:

- Air temperature inside the box (Tₐ)
- Surface temperature inside the box (Tₛ)
● Temperature between the sheet of PMMA and the sheet of PVC ($T_{mr}$)
● Surface temperature outside the box ($T_{so}$)
● Air temperature outside the box ($T_{ao}$)
● Surface temperature inside the heat flux sensor ($T_{sih}$)
● Temperature between the sheet of PMMA and the heat flux sensor ($T_{mh}$)
● Surface temperature outside the heat flux sensor ($T_{soh}$).

The EPS box has the following dimensions: a length of 600mm ±2mm, a width of 400mm ±2mm, a height of 190mm ±2mm and a thickness of 21mm ±1mm. The sheet of PMMA has a thickness of 10mm ±0.1mm and the reference sheet of PVC has a thickness of 4.1mm ±0.05mm as can be seen in Figure 1.

![Figure 1: setup of the experiment](image)

2.2. Procedure

The thermal conductivity of PMMA is to be determined in three different ways: the use of Fourier’s Law of Conduction, the DTA-method and a computer simulation. For the first two methods the experiment needs to be conducted and run until a stationary situation has been reached. The initial temperature of the experiment is 24.4°C and, over a period of 8000 seconds, the heat source shall produce 41.3Js$^{-1}$. The values of the temperatures and those of the heat flux sensor will be recorded by the data logger every 5 seconds.

![Figure 2: histogram showing the frequency of certain air temperatures inside the box](image)

![Figure 3: graph showing the development of certain temperatures over time](image)

The histogram of Figure 2 shows that the last 500 measurements of the air temperature inside the box are all over 48°C. From Figure 3 it can be seen that during the last 1000 seconds of the experiment, all lines depicting the temperatures have almost plateaued entirely, indicating a stationary situation. Therefore, the last 200 measurements will be used to calculate the thermal conductivity of PMMA using both Fourier’s Law and the DTA-method.

For the final method, the experiment is recreated using a simulation software program, wherein it shall be explored whether the simulation is a valid method to determine the thermal conductivity of a material. Like the other experiments, the simulation shall feature a heat source, situated within a box, producing 41.3Js$^{-1}$ for 8000 seconds, as described in the materials section above. The thermal conductivity of PMMA, as calculated in the previous two methods, shall be used, and the resulting temperatures will be compared to those of the conducted experiment.

3. Experiment and simulation
3.1. Fourier’s law of conduction

Fourier’s law of conduction will be applied with the use of the heat flux sensor installed within the experiment. The average heat flux $e$, over the last 1000 seconds, as measured by the heat flux sensor, is $5.27 \text{mV} \pm 0.063 \text{mV}$ (1.2%). Multiplying this figure with the calibration value $C$ of $21.5 \text{Wm}^{-2}\text{mV}^{-1} \pm 1.08 \text{Wm}^{-2}\text{mV}^{-1}$ (5%) as shown in formula (1):

$$q = e \cdot C$$  \hspace{1cm} (1)

results in a heat flux density $q$ of $113.23 \text{Wm}^{-2} \pm 7.023 \text{Wm}^{-2}$ (6.2%). To calculate the total heat flux $Q$ through the PMMA, the heat flux density has to be multiplied by the surface area $A$, according to formula (2):

$$Q = A \cdot q$$  \hspace{1cm} (2)

The surface area $A$ is $0.24 \text{m}^2 \pm 0.002 \text{m}^2$ (0.8%) resulting in a heat flux $Q$ of $27.2 \text{W} \pm 1.1 \text{W}$ (7%) through the PMMA. The thermal resistance $R$ is dependent on the average temperature difference the sheet has generated over the last 1000 seconds: $43.57^\circ\text{C} \pm 0.1^\circ\text{C}$ (0.2%) -- $36.97^\circ\text{C} \pm 0.1^\circ\text{C}$ (0.3%) = $6.60^\circ\text{C} \pm 0.2^\circ\text{C}$ (1.3%). This can be seen in formula (3):

$$R = \frac{\Delta T}{q}$$  \hspace{1cm} (3)

This results in a thermal resistance $R$ of $0.0583 \text{m}^2\text{KW}^{-1} \pm 0.0044 \text{m}^2\text{KW}^{-1}$ (7.5%). To determine the thermal conductivity $\lambda$ of the material, the thickness $d$ of $10 \text{mm} \pm 0.1 \text{mm}$ (1%) as given in the methodology, should be divided by the thermal resistance $R$ as shown in formula (4):

$$\lambda = \frac{d}{R}$$  \hspace{1cm} (4)

The thermal conductivity of PMMA as calculated using Fourier’s law of conduction and the heat flux sensor is $0.171 \text{Wm}^{-1}\text{K}^{-1}$ with an inaccuracy of 8.5% or $0.015 \text{Wm}^{-1}\text{K}^{-1}$.

3.2 DTA-method

Another way to determine the thermal conductivity of PMMA is by using the differential thermal analysis (DTA)-method. This method involves the comparison of the material to be studied with that of another material whose properties are commonly and widely known. The selected reference material used in this experiment was a circle-shaped sheet of polyvinyl chloride (PVC) with a diameter of $14.0 \text{mm} \pm 0.05 \text{mm}$ (0.4%) and a thickness $d$ of $4.1 \text{mm} \pm 0.05 \text{mm}$ (1.2%).

Both the sheet of PMMA and the sheet of PVC will go through identical thermal cycles—they will both be heated up for 8000 seconds by a $41.3 \text{Js}^{-1}$ source. Comparing the results of these cycles leads to a correlation coefficient of 0.939. The lines representing the temperature rise in both materials have a similar shape, as depicted in Figure 4. A difference can be found with regard to a delay in the temperature rise of the PVC, which can be explained by the material being on top of the PMMA sheet, which—until that point in time—had not transferred a noticeable amount of energy. It can be stated that the cycle was almost identical and therefore, that the DTA-method can be applied.

![Figure 4: graph showing the difference in development of temperatures between PMMA and PVC](image-url)
The widely-accepted thermal conductivity $\lambda$ of PVC is $0.17 \text{Wm}^{-1}\text{K}^{-1} \pm 0.02 \text{Wm}^{-1}\text{K}^{-1}$ (11.8%). Using formula (4) the thermal resistance $R$ can be calculated as $24.1 \text{m}^2\text{KW}^{-1} \pm 2.0 \text{m}^2\text{KW}^{-1}$ (8.3%). The thermal resistance $R$ of the sheet of PMMA is proportional to the thermal resistance $R$ of PVC in relation to their average temperature differences $\Delta T$, resulting in a thermal resistance $R$ of PMMA of $6.48 \times 24.1 \times 2.83 = 55.2 \text{m}^2\text{KW}^{-1} \pm 10.2 \text{m}^2\text{KW}^{-1}$ (18.5%). Dividing this by the thickness $d$ of the material according to formula (3) leads to a thermal conductivity of PMMA of $0.18 \text{Wm}^{-1}\text{K}^{-1} \pm 0.035 \text{Wm}^{-1}\text{K}^{-1}$ (19.7%).

3.3 Simulation

Comsol-software was used in order to determine whether a computer simulation is able to simulate the procedure of the experiment accurately by producing the same results. The setup of the experiment is recreated within the software program using all the relevant properties and dimensions of the materials. The thermal conductivity, density and specific heat capacity of the materials EPS, PMMA, PVC and air are filled in, and the initial temperature is set at 24.4°C. For the thermal conductivity of PMMA, the result of the first method—Fourier’s law of conduction—is used because it is the most accurate result: $0.17 \text{Wm}^{-1}\text{K}^{-1}$. Furthermore, the energy produced by the heat source and the time stretch of the simulation are also included.

![Figure 5: temperature development of the experiment as simulated](image1)

The temperature rise of the simulation can be seen depicted in Figure 5. Here, the blue line indicates the air temperature inside the box $T_a$, the green line represents the surface temperature inside the box $T_s$ and the red line shows the surface temperature outside the box $T_o$. The graph initially shows a steep rise in temperature which slowly declines into a gradual rise. After about 7000 seconds the lines begin to plateau and the situation may be described as stationary. The air temperature inside the box has reached about 75°C by this point; the surface temperature remains at 64°C, and the surface temperature outside the box is 45°C. The heat distribution of the simulation can be seen in Figure 6.

4. Comparison and discussion

The thermal conductivity of PMMA, as determined by Fourier’s Law and the DTA-method are very similar, and fall well within each other’s degree of inaccuracy. The former gives a result of $0.171 \text{Wm}^{-1}\text{K}^{-1}$ with an inaccuracy of 8.5% or 0.015 Wm$^{-1}$K$^{-1}$; while the latter results in $0.18 \text{Wm}^{-1}\text{K}^{-1}$ with an inaccuracy of 19.7% or 0.035 Wm$^{-1}$K$^{-1}$. Between the two methods there is, however, a great difference in accuracy: with the determination using Fourier’s law being more than twice as accurate.

The results of the simulation are quite unlike the results of the experiment in their maximum values, with the simulation reaching temperatures as high as 75°C. However, the shape of the two graphs, as depicted in Figure 7 and Figure 8 are quite similar, representing a similar heating cycle.

![Figure 7: temperature development of the experiment as simulated](image2)

![Figure 8: temperature development of the experiment as tested](image3)

The difference between the maximum air temperature as recorded by the simulation and the experiment inside the box is 75°C - 49.5°C = 25.5°C; or 51.5% of the temperature recorded in the experiment. The difference between the surface temperatures inside the box is 64°C - 42.8°C = 21.2°C or 49.5%, and the difference between the surface temperatures outside the box, is 45°C – 33.5°C = 34.3°C or 34.3%.
The difference in recorded temperatures between that of the experiment and that of the simulation can most likely be explained as a result of certain factors not taken into account within the simulation. As previously described, heat transfer takes place via conduction, convection and radiation. The simulation—being a highly simplified model of reality—most likely failed to take into account the heat loss due to radiation. Furthermore, within a real-life situation, there is an almost infinite amount of cooled air supply, resulting in the air temperature outside the box to remain almost unchanged. Therefore, the general recorded temperature rise in the experiment was far lower than that of the simulation.

5. Conclusion

The aim of this study was to explore methods to determine the thermal conductivity of PMMA and to demonstrate which method was more accurate when measuring the thermal conductivity of PMMA. To achieve this aim, several methods of determining the thermal conductivity of PMMA have been investigated and their advantages and limitations addressed. As a result, three methods have been applied: Fourier’s law of conduction with the use of a heat flux sensor, the DTA-method and computer simulation. From the effort of these methods, we may draw the following conclusions:

1. The thermal conductivity of PMMA can be more accurately determined by applying Fourier’s law with the use of a heat flux sensor when compared to the DTA-method. This is mainly the case because of the inaccuracy of thermal conductivity of the reference material, which, if a more precisely known material would be chosen, could result in a much more accurate determination of the thermal conductivity of PMMA.

2. Although the computer simulation does not require a real-life experiment to take place—thereby removing the possibility of human error within the experiment’s calibration and other external factors that could potentially interfere with the data—the results of the simulation were nevertheless seen to differ from that of the real-life experiment. As previously explained, this is most probably the result of the simulation program not taking all possible factors into account. To improve the simulation results in further research the use of a more complex and comprehensive simulation software is recommended, although such programs often have their own limitations, generally being less accessible than the simulation program being used within this research.

Therefore it may be concluded that, regardless of advancements made in measuring thermal conductivity throughout the last century, Fourier’s law remains the most accurate means of determining the thermal conductivity for PMMA.

Nevertheless, the research author would recommend that additional research is conducted in this field, particularly with regard to comparing the application of Fourier’s law with a more accurate and comprehensive simulation software program.

Acknowledgements

The author would like to acknowledge support from the tutors.

References