The computational study of heat conduction in laboratory using Crank-Nicolson finite difference method

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Abstract. The main propose of this research is to study the heat conduction of an aluminium metal bar in an undergraduate thermodynamics laboratory by using the Crank-Nicolson scheme of finite difference method. Heat conduction was simulated to find the thermal conductivity and was compared with the data obtained from the experiment and theory. In the performed boundary and initial conditions, it was found that the predicted thermal conductivity from the simulation was in agreement with those from the theory, however, it was slightly different from the experiment. These results can be used to improve method to find the thermal conductivity in the laboratory more accurately in the laboratory. Besides, these computational approaches can be an optional teaching method for studying thermal conduction for undergraduates, especially for a laboratory that has limited instruments.

1. Introduction
Heat conduction plays important roles in daily life, especially for the conduction of metal or solid materials. The mechanism of this process is that the heat can be transferred in the material through its atoms in which the movement of the atoms is not required [1]. Thermal conductivity $k$ is used to classify the thermal properties of the materials. The detection of $k$ requires instruments which are usually expensive. The laboratory that has limited instruments would not be able to do the experiment of thermal conduction mechanism.

In the heat conduction mechanism, temperature at a position $x$ and time $t$, defined as $u(x,t)$ is explained [2] by heat equation

$$\frac{\partial u(x,t)}{\partial t} = \beta \frac{\partial^2 u(x,t)}{\partial x^2}. \quad (1)$$

When the material is aluminium (Al), $k$ is 238 W/m·°C [3], specific heat capacity $c_p$ is 900 J/kg·°C [3], density $\rho$ is $2.7 \times 10^3$ kg/m$^3$ [3] and diffusion constant $\beta$ is defined as

$$\beta = \frac{k c_p}{\rho}. \quad (2)$$

In 1993, Ozisik [4] proposed simulation results of $k$ by using an implicit backward scheme of finite difference method (FDM) in parallel with $k$ determination from experiment. The research provided a comprehensive understanding for heat conduction in a metal to professionals, however it may be complicated for the beginning undergraduate students. The Crank-Nicolson scheme, FDM, was
proposed to teach a student in parallel with the experiment using basic instruments in a thermodynamic laboratory. These methods not only provide a deep understanding of the mechanism, but also provide the optional method for a limited instrument laboratory.

2. Material and method
In order to study the heat conduction following equation (1), the study was divided into two parts, i.e. experiment and simulation. To initiate the simulation, some parameters, for example, heat rate and the dimension of the aluminium bar, was taken from the experiment. The predicted temperature based on input thermal conductivity was simulated. The temperature was then compared with those measured from the experiment. If the temperature error was within 10% compared to the experiment, the parameters, including the thermal conductivity were accepted. These methods of evaluation are shown as the flow chart diagram in figure 1.

![Figure 1. The flow chart diagram of the heat conduction simulation in a bar.](image)

2.1. Heat conduction experiments
Heat conduction experiments were set up by using conventional instruments in the laboratory as shown in figure 2. The instruments were a metal bar connected by a light plastic string to a stand, beaker, thermocouple, hot plate, thermometer, and a smart phone for time and temperature recording. The 2.004 × 2.004 × 5.600 cm³ of Al metal bar was used to study thermal conductivity. It was isolated except for the bottom side and the conduction side. The bottom side was in contact to temperature source, while the conduction side was left uncovered for observing temperature change. The temperature is measured by the thermocouple attached at one cm from the bar end as shown in the figure 3. A known mass $M_i$ of 200 ml water in 600 ml beaker was heated by a hot plate until the temperature was 98 °C, close to 100 °C, the water vapor temperature. After reaching 98 °C, the beaker was covered by a lid which had a hole in the middle. The Al bar was placed on the top of the hole. In this study, the vapor was then considered as a temperature source to heat the bar until the bar temperature was at maximum stable. The initial time $t_i$ was selected at $T = 35$ °C and final time $t_f$ was at the maximum stable temperature, which usually was 94-95 °C. The remaining water in the beaker was measured as $M_f$. The mass difference $\Delta M = M_f - M_i$ is used to calculate the required latent heat rate $Q$ (W) for this bar volume as

$$Q = \frac{\Delta ML_v}{\Delta t},$$

where $L_v$ is the latent heat of vaporization, 2.26 × 10⁶ J/kg [1], and $\Delta t = t_f - t_i$. The heat rate per area $q_0$ (W/m²) for one second [1] is then calculated according to equation (4) to acquire initial parameters in the simulation.
\[ q_0 = \frac{k(T_h - T_c)}{L}, \]  

where \( T_h \) and \( T_c \) are the temperature in hot and cold region at the bar end, 100 °C and 35 °C, respectively. \( L \) is the bar length, 5,600 cm. In experiment, the thermal conductivity \( k_e \) can be calculated from \[ k_e = \frac{Q L}{A(\Delta T)}, \]  

where \( \Delta T = T_f - T_i \). The experiment was repeated three times. After ending each experiment, \( k_e \) was calculated. The average \( k_e \) was calculated from three experiments and adjusted such that the average \( k_e \) could provide the %error \( \varepsilon_e \) less than 10% compared to the accepted thermal conductivity \( k_{th} \), which was 238 W/m°C [3]. \( \varepsilon_e \) is calculated as

\[ \varepsilon_e = \left| \frac{k_{th} - k_e}{k_{th}} \right| \times 100. \]  

**Figure 2.** The experimental setup for heat conduction study of Al metal bar. The water vapor from beaker on the hot plate is used to heat the bar. During the heat conduction, real time temperature is detected by the thermocouple controller.

**Figure 3.** The bar is connected by a light plastic string to a stand. The bottom side and the front side of the bar are not covered by insulator because they are designed for heat transfer and the thermocouple attachment at one cm from the top, respectively.

2.2. Heat conduction simulation

Heat conduction simulation was initialized by using the adjusted \( q_0 \) from the previous section. The temperature \( u_{(x,t)} \) in the conduction is described by the heat equation [2, 4] in equation (1). The equation can be written as

\[ u_t = \beta u_{xx}, \]  

boundary condition, \(-k \frac{\partial u_{(0,t)}}{\partial x} = q_0, \ x = 0, \ t > 0, \ \frac{\partial u_{(L,t)}}{\partial x} = 0, \ x = L, \ t > 0,\)  

initial condition, \( u_{(x=5,0)} = 35 \ °C, \ x = 5 \ \text{cm}, \ t = 0 \) and \(-k \frac{\partial u_{(x,0)}}{\partial x} = q_0, \) for \( t = 0 \) in \( 0 \leq x \leq L \)
In Crank-Nicolson scheme FDM, for \( u_{i,j}(x,t) = u_j^i \), where subscripts \((i, j)\) represent time and position indices, the time derivative \(u_t\) and the second derivative \(u_{xx}\) are defined as follows:

\[
u_t = \frac{u_{j+1}^i - u_j^i}{h} \quad \text{and} \quad u_{xx} = \frac{(u_{j+1}^{i+1} - 2u_j^i + u_{j-1}^i + u_{j+1}^{i+1} - 2u_j^{i+1} + u_j^{i+1})}{2h^2},
\]

(10)

where \(m\) and \(h\) are time interval and position interval [5]. Substitute these equations into the heat equation in (7), they can be rearranged to be

\[
-\gamma u_{j-1}^{i+1} + (2 + 2\gamma)u_j^{i+1} - \gamma u_{j+1}^{i+1} = \gamma u_{j-1}^i + (2 - 2\gamma)u_j^i - \gamma u_{j+1}^i,
\]

(11)

where \(\gamma\) is defined as

\[
\gamma = \beta \frac{m}{h^2}.
\]

(12)

The conduction was simulated using the input \( q_0 \) from the experiment and using input \( k \) as the same as that of the theory. For simplicity, the dimension of the bar is \(2 \times 2 \times 6 \text{ cm}^3\). The total time was 420 s. While \(m\) and \(h\) were 70 s and 0.01 m, therefore both \(i\) and \(j\) run from 1 to 7. After using the equation (11), with the defined boundary condition and initial condition, temperature \(u_{(x=5 \text{ cm}, t=280 \text{ s})} = T_s\) was known. At \(t = 280\) s, the %error \(\varepsilon\) of the input \(k\) was calculated as a comparison between the simulated temperature \(T_s\) and the experimental temperature \(T_{e280}\) which was measured at \(x = 5.0\) cm and \(x = 4.6\) cm using the equation

\[
\varepsilon_T = \left| \frac{T_s - T_{e280}}{T_s} \right| \times 100,
\]

(13)

where, in this simulation, the parameters were acceptable if they provided \(\varepsilon_T \leq 10\%\).

3. Results and discussion
The results were divided into two parts, experimental results and computational results.

3.1. The experimental results of heat conduction.
The heat conduction experiments were performed as explained in the section 2.1. The top bar end was isolated or set as a boundary region for the simulation purpose. Therefore, temperature of the bar \(T_e\) was detected by the thermocouple attached at one cm from the top. At the beginning of experiment, \(T_e\) was approximately 28 °C. It was slightly increased when the water temperature was increased. After the water temperature measured at 98 °C, the water vapor was moved to heat the bar. As \(T_e\) reached 35 °C, the time at this moment was considered as \(t_i\). After the final time \(t_f\), experimental parameters of those three tests were observed and shown in the table 1. The heat rate \(Q\) and \(k_e\) were calculated based on the parameters according to equation (3) and equation (5). It was found that the average \(Q\) and \(k_e\) with their standard deviation were 380 ± 41 W and 892 ± 107 W/m°C. When compared the average \(k_e\) to \(k_{sh}\), it was found that the %error \(\varepsilon\) was much greater than 10%. The average \(k_e\) was then adjusted by multiplication of 0.25 factor to the heat rate \(Q\). In other words, the adjusted heat rate is

\[
Q_a = 0.25Q.
\]

(14)

Subsequently, the adjusted average \(k_e\) became

\[
k_{ea} = 0.25k_e,
\]

(15)
and provided the average $\varepsilon_x$ as 6.3%, which is less than 10%. The shifting of the measured thermal conductivity from the theory value indicated that the heat rate from the vapor was not entirely used as the heat source. Only 25% of the vapor energy could provide the thermal conduction from 35 °C to 95 °C. A large amount of energy loss, the 75% vapor energy, was expelled to environment rather than directly through the bar for heat conduction.

Table 1. Experimental parameters, the calculated heat rate, conductivity and the adjusted parameters.

| No | $M_i$ (g) | $M_f$ (g) | $\Delta M$ (g) | $T_i$ (°C) | $T_f$ (°C) | $\Delta T$ (s) | $\Delta t$ (s) | $Q$ (W) | $Q_a$ (W) | $k_e$ (W/m ⋅°C) | $k_ea$ (W/m ⋅°C) | $T_{e280}$ (°C) |
|----|---------|---------|--------------|---------|---------|--------------|--------------|--------|--------|----------|-------------|----------|
| 1  | 414.20  | 299.25  | 114.95       | 35.0   | 94.4    | 59.4         | 643.20       | 403.9  | 101.0  | 948     | 237         | 91.4     |
| 2  | 416.05  | 316.55  | 99.50        | 35.1   | 93.7    | 58.7         | 558.00       | 403.0  | 100.7  | 957     | 239         | 92.0     |
| 3  | 418.45  | 377.15  | 41.30        | 35.0   | 95.5    | 60.5         | 280.20       | 333.1  | 83.3   | 768     | 192         | 95.5     |
| Mean | 416.23  | 330.98  | 85.25        | 35.0   | 94.5    | 59.5         | 493.80       | 380.0  | 95.0   | 892     | 223         | 93.0     |
| Std. | 2.13    | 40.91   | 38.84        | 0.06   | 0.91    | 0.91         | 189.82       | 40.61  | 10.15  | 107     | 26.85       | 2.21     |

3.2. The computational results of heat conduction.

Heat conduction of the bar was simulated according to the flow chart diagram in figure 1. The initial heat source to the bar, the heat rate per area $q_0$, had to be carefully selected. As it was found from the experiment that 75% of heat energy had been lost to environment, therefore, the average heat rate per area $q_0$ in equation (4) was input into simulation by multiplying the 0.25 factor. Moreover, it was reduced by a factor of three which accounted for one dimensional conduction. In other words,

$$q_{0a} = \frac{0.25q_0}{3}. \quad (16)$$

$q_{0a}$ from equation (16) was found to be 23,201 W/m$^2$. The results from the simulation based on the input $q_{0a}$ are shown in figure 4. The simulation temperature was slightly increased when the position approach to the bar’s end, but largely increased when given more time. To validate the simulation result, $T_s$ the simulation temperature at $x = 5.0$ cm and $t = 280$ s was collected and found to be 88.9 °C. It was compared to the experimental temperature $T_{e280}$ which was measured at $x = 4.6$ cm and $t = 280$ s. From table 1, $T_{e280}$ is found to be 93.0 ± 2.2 °C. The results of comparison provided $\varepsilon_T = 4.6\%$, which was less than 10%.

In figure 4, in addition to the predicted temperature compared to $T_{e280}$, a transient behavior of temperature is observed. In the figure, it is found that at $t = t_i = 0$ s, the simulated temperature $T_s$ at the position $x = 0$ cm and $x = 5.0$ cm are 39.9 °C and 35 °C, respectively. The latter was the same as the experimental result $T_e$ measured at ($x = 4.6$ cm, $t = 0$ s) which is 35 °C. The agreement between $T_s$ and $T_e$ reassured the validation of the simulation result based on the boundary and initial conditions. When the time was increased, $T_s$ largely increased. Considering at position $x = 5$ cm, as time increased from 0 s to 280 s, the temperature in the semi logarithm scale was increased from 35 °C to 88.9 °C. This increment indicates that the temperature transient behavior is in an exponential pattern.

Furthermore, the simulation thermal conductivity $k_s$ is 238 W/m⋅°C which is the same as the theory value $k_{th}$, but the thermal conductivity from experiment $k_{ea}$ is $223 \pm 24$ W/m⋅°C as shown in the table 1, which is slightly different from the theory and simulation value. Therefore, the Crank-Nicolson method can be used as a parallel method to enhance undergraduate students’ understanding about
thermal conduction. The resulting errors from the study can be decreased by careful placement of the
thermocouple and the bar. Controlling the heat loss and the simulation by including three-dimensional
conduction would provide more accurate results of the thermal conductivity.

Figure 4. Temperature prediction from the simulation at the position from 0 cm to 6 cm and at the time
0 s to 420 s.

4. Conclusion
The thermal conduction was studied using both experimental method and computational method which
followed the scheme of Crank-Nicolson. It was found that \( k \) was large compared to the theory value;
however, after \( Q \) was reduced by the 0.25 factor, \( k \) could have an error of only 6.3%. The factor was
also multiplied by \( q_0 \) which was used to initiate the temperature change simulation in the bar. After
correction for one dimensional conduction, it was found that the temperature from the simulation was
slightly different from the experiment with 4.6% error. Therefore, it could be concluded that Crank-
Nicolson thermal conductivity simulation in parallel to the basic experiment provided errors less than
10%. The heat conduction mechanism was observed via the change of temperature in an exponential
behaviour. These methods thus could be used to teach undergraduate students in parallel with the
experimental method. For wider application, the methods should be used with other types of metal.
Errors should be decreased for more precision value of \( k \) on any solid material.

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