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A Study and Mathematical Modelling of thermal conductivity of a Thermodynamic System

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Abstract

Theoretical available values of thermal conductivity are commonly different from the experimentally obtained values. In the present work, a thermodynamic system has been considered and variations in temperature in different elements were analyzed and corresponding thermal conductivities were calculated. These values were compared and the corrected values were justified on the basis of a mathematical model made by introducing semi-empirical corrections. The theoretical value of the thermal conductivity of an isolated system (K_T) and the corresponding corrected value were found in agreement with each other.

Key Words: Heat transfer, Methamical model, Thermal conductivity, Thermodynamic system.

1. Introduction

Heat transfer is a common phenomenon in metals and various other engineering materials. In today's world, various thermodynamical systems are explained and analysed on the basis of *observations.* Observations are taken and they are recorded. On these records, phenomenon of heat transfer is analysed. There is no sure shot theoretical and mathematical model to those systems i.e. there is no theoretical basis for this phenomenon. The present paper discusses an experiment and procedure of analysis. The experiment deals with the ancient problem of thermal conduction through a metallic cylinder whose ends sit at temperatures T1 and T2 where T1>T2. The metallic cylinder is of length L and diameter D. Heat conduction occurs from face 1 to face 2. Assuming an isolated system, the heat exchange can be written as [1, 2]:

□Q / □t = -K (A/L)□ □ □................. (1)

Where □Q/□t is the heat transfer per unit time, K is the thermal conductivity of the material, A is the surface area, L is the total length of the cylinder and □ □ □is the temperature difference between the two faces. In this work, an experiment is reviewed that can be used to determine K for different metallic materials where the theoretical model expressed by eqn 1 represents only a first approximation to the reality. The main difference b/w theory and experimental facts is explored in this work in a scientific way.

2. Experimental Procedure

The experimental set up [3] consists of a metallic cylinder (diameter D, and length L) that is used to connect two cups. For all the experiments presented in this work it was always adopted D = 15.85 and L = 61.00 mm. Cup 1 is made of aluminum and it is filled with water (M1 = 300 ml) at room temperature. The water temperature inside Cup 1 is going to be referred as T1, and it is monitored by the use of a thermometer. Cup 2 is made of Teflon, which is filled of ice and water and it weighs M_2. It has also a Teflon cover with a hole for the introduction of a thermometer that is used to monitor the temperature (T2) of a fixed amount of water (M_2) inside Cup 2. A stirrer is used for better temperature homogenization inside cup 2

3. Results and Discussions

3.1. The simplest model

We observed that for the case of a copper, the cylinder takes 800 sec for heating of T2 from 0^oC to 36^oC. For the aluminium this figure is 1350 sec and for brass, it is 1840 sec. In order to determine K using the theoretical model predicted by eqn 1, □Q can be calculated using the approximations that all heat that is transferred from cup1 to cup2. According to that simple model, for each variation of T2 by one degree, □Q can be written as in eqn 2.

□Q = $M_2 C_W$ □T_W .... (2)

Here C_W is the specific heat of water (equal to 1 cal/g ^oC) and $\Delta\theta_W$ is the increase in the temperature equal to 1^oC. For each material, K can be determined by substituting eqn 2 in eqn 1. We name this model as model 1, and thus K is denoted as K_1 and written as in eqn 3.

$$\mathbf{K1 = (M_2\, C_W\, \Delta T_W\, L) / (A\, \Delta T\, \Delta t)} \quad \ldots\ldots\ldots\ldots\ldots \mathbf{(3)}$$

Note that in equation 3 most of the parameters are constants, besides ΔT and Δt (assuming ΔT_W as 1^oC). Figure 2(a) shows the results of K_1 as a function of T2 for copper (squares), aluminum (circles) and brass (triangles) respectively. Three different regions named A, B and C are illustrated in Fig. 2(a), and they are separated by the vertical dashed lines. Each of them will be considered separately next. The data for T2 < 5°C were not shown in region A. They were excluded from the graph because region A represents a regions where the system in not in equilibrium yet (a mixture of water and ice exists inside cup2, that also presents a temperature gradient), thus K1 values start from close to zero and reach the equilibrium value at about T2 equal to 5°C. In this sense, region A is totally disregarded. Regions B and C are separated according to room temperature, that was about 27°C. In fig 2(a), the variation of experimentally obtained thermal conductivity (K1) according to the simplest theoretical model described by eqns. 1 and 2 for three metallic cylinders made of copper (squares), aluminium (circles) and brass (triangles) is plotted as a function of the temperature (T2) inside Cup2. Here vertically dashed lines separate three regions: a) Non-Equilibrium Region; b) Quasi-Equilibrium Region for T2 smaller than room temperature; c) Quasi-Equilibrium Region for T2 higher than room temperature [6]. It can be observed from figure that the experimental K1 is neither constant nor linear as a function of T2. This finding is in total disagreement with the predicted theoretical model. On top of that the experimentally obtained K1 maxima are considerably smaller than those reported for copper [0.92 cal /(°C sec cm)], aluminum [0.49 cal /(°C sec cm)] and brass [0.26 cal /(°C sec cm)] [8]. The difference between reported and experimentally determined values is bigger, the higher the reported K value [7].

3.2 The influence of Teflon Cup

The model needs a correction in region B because the total increase in T2 is due to the heat conduction through the metallic cylinder ($\Delta Q_{CYLINDER}$), plus the heat conduction from the Teflon Cup (ΔQ_{CUP}). In this sense, the total heat transferred to the water inside Cup 2 can be written as

$$\mathbf{\Delta Q_{WATER} = \Delta Q_{CYLINDER} + \Delta Q_{CUP}} \quad \ldots\ldots\ldots\ldots\ldots \mathbf{(4)}$$

$\Delta Q_{CYLINDER}$ calculated from eqn 4 can be substituted into eqn 1. ΔQ_{WATER} is calculated as in eqn 4 and ΔQ_{CUP} is calculated in eqn 5

$$\mathbf{\Delta Q_{CUP} = (K_{TE}\, A_{TE} / d_{TE})\, \Delta\theta_{TE}\, \Delta t} \quad \ldots\ldots\ldots\ldots\ldots\ldots \mathbf{(5)}$$

where Δt is the same time interval as before, ΔT_{TE} is the temperature difference between the internal and external walls of the teflon cup, d_{TE} is the thickness of the walls of the cup (7.5 mm), K_{TE} is the thermal conductivity of teflon (4.53 X 10^{-4} cal/(^oC s cm)) and A_{TE} is the effective area of the cup in contact with the water inside it. This area can be written as the sum of lateral and the bottom areas and can be approximated by the eqn 6 using an average cup radius R_{TE} (37.2 mm)

$$\mathbf{A_{TE} = 2\pi\, R_{TE}\, H + \pi R_{TE}^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots \mathbf{(6)}$$

where H is the height of the water column inside Cup 2 (76.1 mm). Note that the cup is not in contact with the water inside it. According to the above, the $\Delta Q_{CYLINDER}$ to be used in eqn 1 would be given by equation 7.

$$\mathbf{\Delta Q_{CYLINDER} = M_2 C_W \Delta\theta_W - \{(K_{TE}/d_{TE})(2\pi R_{TE} H + \pi R^2_{TE})\, \Delta\theta_{TE}\, \Delta t\}} \quad \ldots\ldots\ldots\ldots \mathbf{(7)}$$

This suggests an even worse result than the one observed in Eqn. 3, given that a smaller $Q_{CYLINDER}$ would be obtained. The total heat through the cylinder is used in increasing the water temperature inside Cup 2 (ΔQ_{WATER}), cup temperature (ΔQ_{CUP_A}) and remaining portion is lost in heat transfer through Cup 2 to the atmospheric environment (ΔQ_{CUP_B}). Thus, $\Delta Q_{CYLINDER}$ can be written as

$$\mathbf{\Delta Q_{CYLINDER} = \Delta Q_{WATER} + \Delta Q_{CUP\_A} + \Delta Q_{CUP\_B}} \quad \ldots\ldots\ldots\ldots\ldots \mathbf{(8)}$$

Here ΔQ_{WATER} is calculated as in Eqn.2 and ΔQ_{CUP_B} is calculated as in equation 5. In order to calculate ΔQ_{CUP_A} it is assumed a linear temperature distribution though the thickness of the Teflon cup as illustrated by the solid line in Fig. 3(a). It is also assumed that for each Δt the temperature distribution varies qualitatively according to the dashed line. According to these approximations, the total heat stored inside the cup material itself would be

$$\mathbf{\Delta Q_{CUP\_A} = \int_0^{dTE} \rho_{TE}\, A_{TE}\, C_{TE}\, \Delta\theta(x)\, dx = \rho_{TE}\, A_{TE}\, C_{TE} \int_0^{dTE} \Delta\theta(x)\, dx} \quad \ldots\ldots\ldots \mathbf{(9)}$$

Here ρ_{TE} is the mass density of Teflon (2200 kg/m^3), A_{TE} is given by equation 6, C_{TE} is the specific heat of Teflon (0.28 cal/ (g ^oC)), and $\Delta T(x)$ is the temperature variation inside the thickness of the cup as a function of the length.. In fig 3(a), T_{EXT} is the external temperature; T_{INT-1} and $_{TINT-2}$ are the internal initial and final temperatures respectively. In fig 3(b), T1 is the constant temperature of cup1; T_{2-i} and T_{2-f} are the initial and final temperatures of Cup2 respectively. The solid line (numerically numbered 1) represents the initial temperature distribution and the dashed line (numbered 2) represents the final temperature distribution after the time interval t for both curves. This information can be extracted from Fig. 3(a) [9] using the difference between the two equations that describe each of the linear dependence of T with x before and after Δt. According to that, the initial distribution of temperature is

$$\mathbf{T1(x) = T_{INT-1} - a1.x} \text{ with } \mathbf{a1 = (T_{INT-1} - T_{EXT})/d_{TE}} \quad \text{………… (10)}$$

And the final distribution temperature after Δt elapsed is

$$\mathbf{T2(x) = T_{INT-2} - a2.x} \text{ with } \mathbf{a2 = (T_{INT-2} - T_{EXT})/d_{TE}} \quad \text{……………. (11)}$$

Using eqn 10 and 11, $\Delta T(x)$ can be written as

$$\mathbf{\Delta T(x) = T2(x) - T1(x) = T_{INT-2} - T_{INT-1} + \{(T_{INT-1} - T_{INT-2})/d_{TE}\}\ x} \quad \text{…………. (12)}$$

Taking into account that the variation from T_{INT-1} to T_{INT-2} is equal to 1^0C, eqn 12 can be written as $\mathbf{\Delta T(x) = 1 - (x/d_{TE})}$ ………….. **(13)**

The substitution of eqn 13 into eqn 9 leads to

$$\mathbf{\Delta Q_{CUP\_A} = \rho_{TE} A_{TE} C_{TE} \int_0^{d_{TE}} (1 - x/d_{TE})\, dx = \rho_{TE} A_{TE} C_{TE} (d_{TE} / 2)} \quad \text{………….. (14)}$$

Then the expression for $\Delta Q_{CYLINDER}$ can be obtained by substituting eqn 2, 5 and 14 into eqn 8

$$\mathbf{\Delta Q_{CYLINDER} = M_2C_W \Delta\theta_W + \{(K_{TE} /d_{TE}) (2\pi R_{TE}\, H + \pi R^2{}_{TE}) \Delta T_{TE}\, \Delta t\} + \rho_{TE} A_{TE} C_{TE} (d_{TE} /2)} \quad \text{……. (15)}$$

3.3. Losses through cylinder

Two other different mechanisms exist, besides the heat conduction from cup1 to cup2 by the metallic cylinder. The first of them regards the heat that is lost through the surface of the cylinder (ΔQ_{SURF}) in its radial direction, i.e. along the vertical arrow in Fig. 1 because, in principle, each section of the cylinder sits at a temperature T higher than room temperature. The second mechanism regards the storage of heat inside the metallic cylinder itself (ΔQ_{STORED}) as previously described for Cup 2 [5]. In this sense, the total heat lost (ΔQ_{LOST}) can be written as

$$\mathbf{\Delta Q_{LOST} = \Delta Q_{SURF} + \Delta Q_{STORED}} \quad \text{………….. (16)}$$

The heat lost through the surface ΔQ_{SURF} is one of the most difficult to be quantified, mainly because of its three-dimensional character. As a very rough approximation, it could be said that the heat transfer rate at each section of the cylinder (i.e. in its radial direction) would be given as

$$\mathbf{\Delta(\Delta Q_{SURF}/\Delta t) = -K\ (A_{SEC}/L_{SEC})\ \Delta T(x)\ \Delta x} \quad \text{(17)}$$

Here Δt is the elapsed time as before, K is the thermal conductivity of the metallic cylinder, $\Delta T(x)$ is the temperature difference between the highest temperature inside each section of the cylinder and room temperature, A_{SEC} is an effective area and L_{SEC} is an effective length for the heat transfer, respectively. Just as a simple approximation it could be assumed that A_{SEC} can be approximated by the perimeter of the section at position x, i.e., $A_{SEC} = \pi D$ & the highest temperature inside the section is localized at the cylinder axis, i.e., a linear gradient of temperature will be assumed for each section with the highest temperature value sitting at the cylinder axis and the lowest temperature value sitting at the external surface thus leading to L_{SEC} = D/2. According to the above, ΔQ_{SURF} could be written as

$$\mathbf{\Delta Q_{SURF} = \int_0^{L} (K\ 2\pi D/D) \Delta t\ \Delta T(x)\, dx = 2\pi K\ \Delta t \int_0^{L} \Delta T(x)\, dx} \quad \text{…………… (18)}$$

Note that L in equation 18 refers to the cylinder length between the two cups. In order to solve the above equation $\Delta T(x)$ must be known. Applying the same approximation as in the previous section

$$\mathbf{T_{INT} = T1- ax} \text{ with } \mathbf{a= (T1-T2)/L} \quad \text{……………… (19)}$$

Then ΔQ_{SURF} can be finally written as:

$$\mathbf{\Delta Q_{SURF} = 2\pi K\ \Delta t \int_0^{L} (T1-T_{EXT}) - \{(T1-T2)/L\}\ x\ dx = 2\pi KL\ \Delta t\ \{T1-T_{EXT} - (T1-T2)/2\}} \quad \text{……… (20)}$$

On the other hand, the heat stored inside the cylinder itself ΔQ_{STORED} can be calculated using the same procedure as before for the case of Cup 2. The only difference now is the fact that the temperature distribution inside the cylinder and its variation after Δt would be illustrated by figure 2(b). According to figure 2(b), $\Delta T(x)$ can be written as

$$\Delta T(x) = T1 - (T1-T2\_f)\, x/L - \{T1-(T1-T2\_i)\, x/L\} = x/L\, (T2\_f - T2\_i) = x/L \quad \ldots\ldots\ldots\ldots (21)$$

because the difference between T2_f and T2_i is always kept equal to 1°C. The heat stored in each section of the metallic cylinder can be written as

$$\Delta Q(x) = \rho_M\, \pi\, (D/2)^2\, C_M\, \Delta T(x) \quad \ldots\ldots\ldots\ldots (22)$$

where ρ_M and C_M are the mass density and specific heat of the metallic cylinder, respectively. For Brass, the value of ρ_M (C_M) is equal to 8400 (0.090). For Aluminium, it is 2700 (0.215) and for Copper, it is 8920 (0.092) kg/m^3 (cal/(g °C)). After the substitution of eqn 21 into 22, the total stored heat can be calculated,

$$\Delta Q_{STORED} = \int_0^L \rho_M\, \pi (D/2)^2\, C_M\, (x/L)\, dx = \rho_M\, \pi (D/2)^2\, C_M\, (L/2) \quad \ldots\ldots\ldots (23)$$

The substitution of eqn 20 and 23 in eqn 16 leads to final ΔQ_{LOST}

$$\Delta Q_{LOST} = 2\pi KL \Delta t\, [T1 - T_{EXT} - (T1-T2)/2] + \rho_M\, \pi (D/2)^2\, C_M\, (L/2) \quad \ldots\ldots\ldots (24)$$

For region B, all contributions add up as

$$\Delta Q_{CYLINDER} = M_2 C_W \Delta T_W - \{(K_{TE}/d_{TE})\, (2\pi R_{TE} H + \pi R^2_{TE})\, \Delta T_{TE}\, \Delta t\} + 2\pi KL \Delta t\, \{T1 - T_{EXT} - (T1-T2)/2\} + \rho_M\, \pi (D/2)^2\, C_M\, (L/2) \quad \ldots\ldots\ldots\ldots (25)$$

The substitution of eqn 25 in 1 would lead final value of K for region B of:

$$K_B = \Psi/Z \quad \ldots\ldots\ldots\ldots (26)$$

$$\Psi = M_2 C_W\, \Delta T_W - \{(K_{TE}/d_{TE})\, (2\pi R_{TE} H + \pi R^2_{TE})\, \Delta T_{TE}\, \Delta t\} + \rho_M\, \pi (D/2)^2\, C_M\, (L/2) \quad \ldots\ldots\ldots\ldots (27)$$

$$Z = (A/L)\, \Delta t\, \Delta T_W - 2\pi L\, \Delta t\, \{T1 - T_{EXT} - (T1-T2)/2\} \quad \ldots\ldots\ldots\ldots (28)$$

For region C contributions in equation 15 and 24 add up as

$$\Delta Q_{CYLINDER} = M_2 C_W\, \Delta T_W + \{(K_{TE}/d_{TE})\, (2\pi R_{TE} H + \pi R^2_{TE})\, \Delta T_{TE}\, \Delta t\} + \rho_{TE} A_{TE} C_{TE}\, (d_{TE}/2) + 2\pi KL \Delta t\, (T1 - T_{EXT} - (T1-T2)/2) + \rho_M\, \pi (D/2)^2\, C_M\, (L/2) \quad \ldots\ldots\ldots (29)$$

The substitution of equation 29 into equation 1 would lead to a final K value for region C

$$K_C = \Psi/Z \quad \ldots\ldots\ldots\ldots (30)$$

$$\Psi = M_2 C_W\, \Delta T_W + \{(K_{TE}/d_{TE})\, (2\pi R_{TE} H + \pi R^2_{TE})\, \Delta T_{TE}\, \Delta t\} + \rho_M\, \pi (D/2)^2\, C_M\, (L/2) + \rho_{TE} A_{TE} C_{TE}\, (d_{TE}/2) \quad \ldots\ldots\ldots\ldots (31)$$

and Z is given by equation 28. These models are based on many approximations. Even though the mathematical models are not accurate, the most important physical mechanisms for heat conduction and heat storage have been identified.

4. Alternative Approach

In order to better understand the system, a different approach can be adopted by a huge turn in the experiment [10]. We can: a) Adopt the reported K values as known constants; b) Introduce a function F (T2) that would represent the correction that must multiply the second term of Z in eqn. 28 for the right answer, thus leading to a new function called Z2; c) Determine F(T2) using expressions 26, 27 and the corrected equation 28. Note that a new semi-empirical model for the second term of equation 28 would be obtained this way. Curiously, after the proper substitution, the obtained F (T2) is a linearly decreasing function of T2 for the three cylinders, i.e., F (T2) = a - b.T2. Fig. 2(b) presents the experimental data for the case of the aluminum cylinder only. In this figure Empirical function F (T2) is shown as a function of the temperature inside Cup2 for the correction of the second term in eqn. 28 for the case of aluminium cylinder. Note that F (T2) is a linear function of T2. The corresponding coefficients of the linear fits for the case of the three metallic cylinders are presented in the inset of Fig. 2(b). Note that each metallic cylinder has its own set of fitted parameters, indicating that the correction function F (T2) is in fact a function of the cylinder material also. The fitted parameters, a and b, are plotted in Fig. 4 as a function of each reported K value, where the cylinder material is also identified. Parameter a is plotted as solid squares, while parameter b is plotted as open triangles. It is also interesting to observe the non-linear variation of both parameters as a function of the reported K value, indicating that once again the cylinder material itself plays a very important role. Note that both a and b parameters increase with K, and that while the ratio of the highest to lowest reported K value is about 3.5, the ratio of highest and lowest a (or b) parameters is less than 2. The final semi-empirical correction to the second term of eqn 28 would depend upon two variables (K and T2) as in eqn 32. Moving to the analysis of region C, the corrected

Z2 term should be used in place of Z in equation 30 as discussed above. The first three terms in equation 31 are basically the same as in equation 27 (the only difference being the fact that the second term is now added rather than subtracted in the whole expression). According to the previous discussion about region B, these terms can be considered mathematically correct, and in this case, the only possibility of disagreement must come from the fourth term in equation 31. The fourth term in equation 31 is more than twice as big as the sum of the other three in the same expression. Thus, it is reasonable to assume that the fourth term has been the overestimated one. The main reason for that is the very simple distribution of temperature inside the walls of Cup2 itself. Following the same procedure as for region B, we can try to determine a function G(T2) that would multiply the fourth term in equation 31, thus leading to a corrected □2 value in substitution to □ in equation 31. Once again, a semi-empirical model would be obtained. In practice, once again the obtained function is linearly dependent on T2, and can be written as G (T2) = c + d .T2. The fitted parameters c and d are plotted in Fig. 4 for the case of the three metallic cylinders. As in the previous case, the fitted parameters depend on the material also and the final G (T2) could then be written as in eqn 33. Fig. 5 shows the final results obtained with Copper, Aluminium and Brass cylinders. The improvement of the semi-empirical model is outstanding.

$$F(T2, K) = a(K) - b(K).T2 \quad \ldots\ldots\ldots\ldots\ldots\ldots.. \quad (32)$$

$$G(T2, K) = c(K) + d(K).T2 \quad \ldots\ldots\ldots\ldots\ldots\ldots.. \quad (33)$$

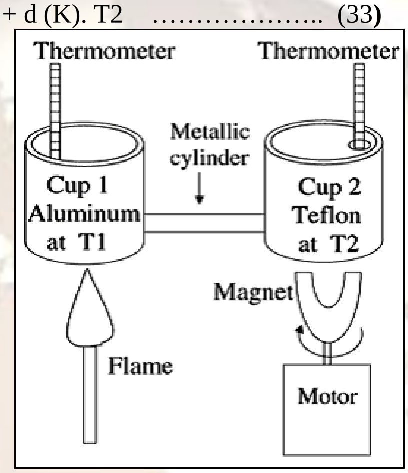

Fig. 1 Experimental Set up

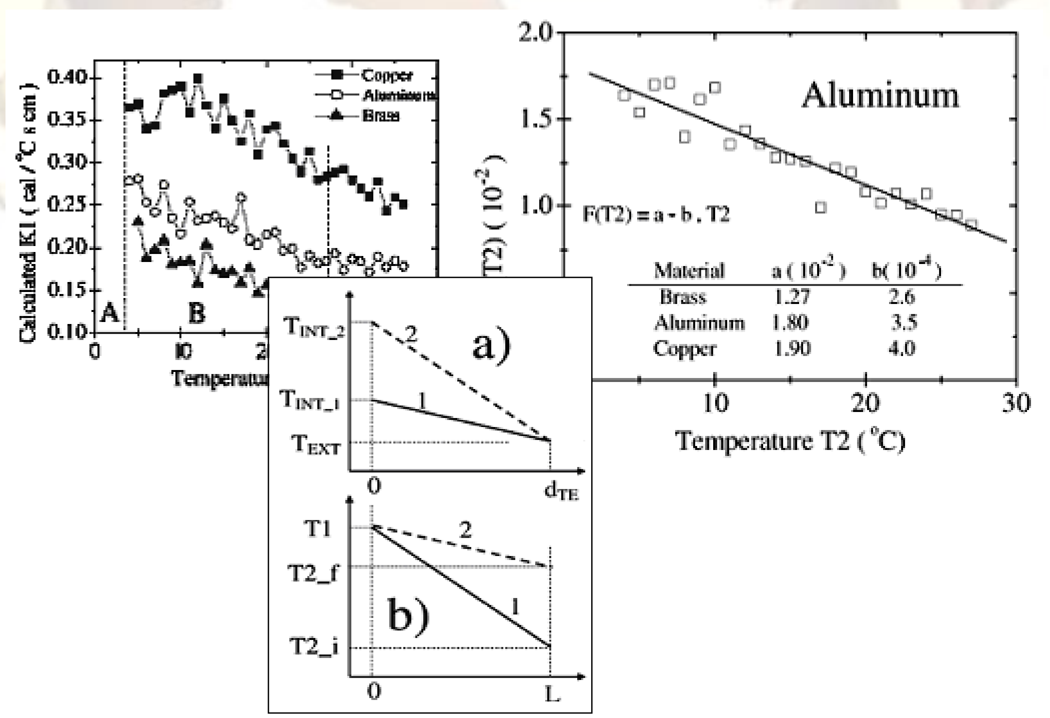

Fig 3 (a) Linear temperature distribution though the thickness of the Teflon cup

(b) Variation of temperature along the extension of the metallic cylinder

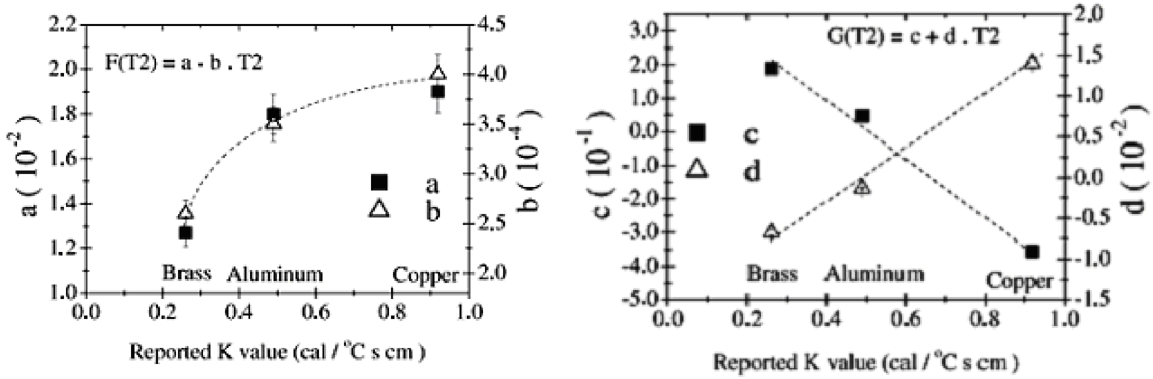

Fig. 4: Variation of fitted parameter (a, b, c and d) with reported value of thermal conductivity

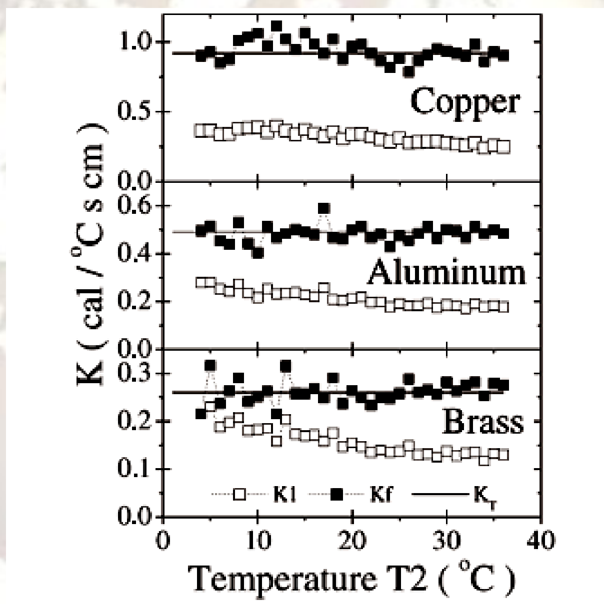

Fig 5: Final model showing the variation of three thermal conductivities (K1, Kf, K_T) with temperature T2

K1 – Thermal conductivity according to eqn.1 assuming isolated system
Kf- Thermal conductivity according to the corrections considered in region B & C
K_T – Reported or literary values of Thermal conductivity

5. Conclusions

The different aspects of the thermal conductivity have been clearly explained. The advantage of introducing the functions F and G in the corrected models was that the temperature distribution inside each section of the cylinder and inside the walls of Cup 2 gets oversimplified. Thus in an isolated system, the experimental region and the region which was corrected theoretically can be compared easily with the aid of figure 5. The theoretical value of the thermal conductivity of an isolated system (K_T) and the corresponding corrected value were found to be lying around each other but they were comparatively higher than the values of K as per eqn. 1.

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